REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, N-phenyl-, reaction product with 2,4,4-trimethylpentene

CAS No. 68411 - 46 - 1

Sponsor Country :

DATE:

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2003 AUG 27 PM 3:07

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 68411-46-1

B. Name *(IUPAC name)*

***C. Name** *(OECD name)*

†D. CAS Descriptor Benzenamine, N-phenyl-, reaction product with 2,4,4-trimethylpentene

E. EINECS-Number 270 -128 - 1

F. Molecular Formula

***G. Structural Formula**

H. Substance Group

I. Substance Remark

J. Molecular Weight 298-350

1.02 OECD INFORMATION

A. Sponsor Country:

B. Lead Organisation:

Name of Lead Organisation: Noveon, Inc
Contact person: Robert K. Hinderer, Ph.D
Address:
Street: 9911 Brecksville Road
Postal code: 44141-3247
Town: Cleveland, Ohio
Country: U.S.A.
Tel: (216) 447-5181
Fax: (216) 447-5760

C. Name of responder

Name:
Address:
Street:
Postal code:
Town:
Country:
Tel:
Fax:

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. Purity

1.2 SYNONYMS Vanlube® 848; Vanox® 1081; Good-rite® 3191; Good-rite® Stalite S; Naugalube® 640; Irganox L 57

1.3 IMPURITIES

CAS No:	122-39-4
EINECS No:	
Name:	Diphenylamine
Value:	3-5%
Remarks:	

1.4 ADDITIVES

CAS No:	
EINECS No:	
Name:	
Value:	
Remarks:	

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT**

Value:	44-107 °C
Decomposition:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	
GLP:	Yes **[ ]** No **[x]** ? **[ ]**
Remarks:	Range for major components; the melting point of the butylated/octylated component could not be determined because it was an oil.
Reliability:	(2) Valid with restrictions
Reference:	Noveon, Inc. Laboratory

***2.2 BOILING POINT**

Value:	>300 °C
Pressure:	at . . . . . hPa

Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: >200° C (Noveon and Uniroyal MSDS's)
Reference: Ciba MSDS

BOILING POINT

Value: Approx. 370 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: 326.04 to 431.62 for major components
Reliability: (2) Valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: EPIWIN

†2.3 DENSITY (relative density)

Type: Bulk density **[ ]**; Density **[x]**; Relative Density **[ ]**
Value: 0.97 +/- 0.01 mg/m3
Temperature: 25 °C
Method:
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Remarks: Specific Gravity 0.96-0.99 (H20=1) (Ciba MSDS)
Reference: Noveon, Inc. MSDS

*2.4 VAPOUR PRESSURE

Value: 2x10(-5) mmHg hPa
Temperature: 25 °C
Method: calculated **[ ]**; measured **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Negligible @ 20 degrees C (Uniroyal MSDS)
Reliability: (2) Valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Ciba MSDS

VAPOUR PRESSURE

Value: 1.14E-004 to 5.05E-008 hPa
Temperature: °C
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for major components
Reference: EPIWIN

*2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$

Log Pow: >>6
Temperature: °C
Method: calculated **[ ]**; measured **[ ]**

GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks:
Reliability: (2) Valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Ciba MSDS

PARTITION COEFFICIENT $log_{10}P_{ow}$

Log Pow: 5.2 to 10.82
Temperature: °C
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for major components
Reference: EPIWIN

*2.6 WATER SOLUBILITY

A. Solubility

Value: <0.01%
Temperature: 20°C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Negligilbe (Noveon, Inc.; Insoluble in water (Uniroyal MSDS)
Reliability: (2) Valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: Ciba MSDS

Solubility

Value: 1.167 to 1.939e-006 mg/l
Temperature: °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for major components
Reference: EPIWIN

2.7 FLASH POINT *(liquids)*

Value: °C
Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.8 AUTO FLAMMABILITY

Value: °C
Pressure: hPa
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;
More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

†2.12 OXIDATION: REDUCTION POTENTIAL

Value: mV
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]** Remarks:
Reference:

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

B. Other data

Results:
Remarks:
Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: nm
Relative intensity:
Spectrum of substance: nm
Concentration of Substance:
Temperature: °C
Direct photolysis:
Half life: 0.053 days
Degradation: % (weight/weight) after . . . . . (exposure time)
Quantum yield:
Type of sensitizer:
Concentration of sensitizer:
Rate constant (radical): cm^3/molecule*sec
Degradation:
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks: Range for major components
Reliability: (2) Valid with restrictions
Reference: EPIWIN

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: . . . . . at pH . . . . . at . . . . . °C
Degradation: . . . . . at pH . . . . . at . . . . . °C after
. . . . . (exposure time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration: .
Soil temperature: °C
Soil humidity:
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year . . . . . .
Content of clay etc.: Clay . . . . . %, Silt . . . . . %, Sand . . . . . %
Organic Carbon:
Soil pH:
Cation exchange capacity:
Microbial biomass:
Dissipation time: DT 50 :
DT 90 :
Dissipation : . . . . . % after . . . . . (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

*3.2 MONITORING DATA (ENVIRONMENTAL)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media:
Results:
Remarks:
Reference:

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media:
Method:
Results:
Remarks:
Reference:

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPIWIN
Results: Air 0.0697%, 1.28 hr half-life, 1000 kg/hr
Water 17.4%, 900 hr half-life, 1000 kg/hr

Soil 49.6%, 900 hr half-life, 1000 kg/hr
Sediment 33%, 3.6e+003 hr half-life, 1000 kg/hr

Remarks:
Reliability: (2) Valid with restrictions
Reference: EPIWIN

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results:
Remarks:
Reference:

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
% after (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) % in (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5
Method:
Concentration: related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: mg O_2/l
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method:
Value: mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD_5/COD:
Remarks:
Reference:

3.7 BIOACCUMULATION

Species:
Exposure period:
Temperature: °C
Concentration
BCF:
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**

Method:
Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Reference:

3.8 ADDITIONAL REMARKS

A. Sewage treatment

Results:
Remarks:
Reference:

B. Other information

Results:
Remarks:
Reference:

4. <u>ECOTOXICITY</u>

***4.1 ACUTE/PROLONGED TOXICITY TO FISH**

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: LC_{50} (24h) = mg/l
LC_{50} (48h) = mg/l
LC_{50} (72h) = mg/l
LC_{50} (96h) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

***A. Daphnia**

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**;
open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: EC_{50} (24h) = mg/l
EC_{50} (48h) = mg/l
EC_{xx} (..h) = mg/l
NOEC = mg/l

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: EC_{50} (24h) = mg/l
EC_{50} (48h) = mg/l
EC_{xx} (..h) = mg/l
NOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

***4.3 TOXICITY TO AQUATIC PLANTS**

Species:
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (h) = mg/l
(Endpoint) EC_{xx} (h) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.4 TOXICITY TO BACTERIA

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:
Exposure Period:
Results: EC_{50} (. . . h) = mg/l
EC_{xx} (. . . h) = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:	
Endpoint:	Length of fish **[ ]**; Weight of fish **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period:	
Results:	. EC_{50} (..d) = mg/l
(Endpoint)	EC_{xx} (..d) = mg/l
	NOEC = mg/l
	LOEC = mg/l
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[ ]**
Method:	
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:	purity:
Remarks:	
Reference:	

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:	
Endpoint:	Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period:	
Results:	EC_{50} (. . . . . h) = ... mg/l
(Endpoint)	EC_{xx} (. . . . . d) = ... mg/l
	NOEC = ... mg/l
	LOEC = ... mg/l
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[ ]**
Method:	
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:	purity:
Remarks:	
Reference:	

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type :	Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species:	
Endpoint:	Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:	
Results:	EC_{50} (. . . . . d) = ... mg/kg
(Endpoint)	EC_{50} (. . . . . d) = ... mg/kg
	EC_{xx} (. . . . . d) = ... mg/kg
	NOEC = ... mg/kg
	LOEC = ... mg/kg
Method:	

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or $LC_{50\ (7d)}$ = ... mg/l
EC_{50} and/or $LC_{50(14d)}$ = ... mg/l
EC_{xx} and/or $LC_{xx\ (xxd)}$ = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

(b)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or $LC_{50\ (7d)}$ = ... mg/l
EC_{50} and/or $LC_{50(14d)}$ = ... mg/l
EC_{xx} and/or $LC_{xx\ (xxd)}$ = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:
(c)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or $LC_{50\ (7d)}$ = ... mg/l
EC_{50} and/or $LC_{50(14d)}$ = ... mg/l
EC_{xx} and/or $LC_{xx\ (xxd)}$ = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: ....., purity: .....
Remarks:
Reference:

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

Results: Substance:
Species or ecosystem studied:
Effects monitored:
Results:
Chemical analysis:
Remarks:
Reference:

4.8 BIOTRANSFORMATION AND KINETICS

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results:
Remarks:
Reference:

4.9 ADDITIONAL REMARKS

Results:
Remarks:
Reference:

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Value: mg/kg b.w.:
Discriminating dose:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**

Species/strain:
Exposure time:
Value:
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 [ ]; LD_{100} [ ]; LD_{50} [ ]; LDL_0 [ ]; Other [ ]
Species/strain:
Value: mg/kg b.w.
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC_0 [ ]; LC_{100} [ ]; LC_{50} [ ]; LCL_0 [ ]; Other [ ]
LD_0 [ ]; LD_{100} [ ]; LD_{50} [ ]; LDL_0 [ ]; Other [ ]
Species/strain:
Route of Administration: i.m. [ ]; i.p. [ ]; i.v. [ ]; infusion [ ]; s.c. [ ]; other [ ]
Exposure time:
Value:
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

.

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain:
Results: Highly corrosive [ ]; Corrosive [ ]; Highly irritating [ ];
Irritating [ ]; Moderate irritating [ ]; Slightly irritating [ ];
Not irritating [ ]
Classification: Highly corrosive (causes severe burns) [ ];
Corrosive (causes burns) [ ]; Irritating [ ]; Not irritating [ ]
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

5.2.2 EYE IRRITATION/CORROSION

Species/strain:
Results: Highly corrosive [ ]; Corrosive [ ]; Highly irritating [ ];

Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**

Classification: Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

5.3 SKIN SENSITISATION

Type: Magnusson & Kligman Maximisation Test
Species/strain: Guinea Pig/Dunkin Hartley
Results: Sensitizing **[ ]**; Not sensitizing **[x]**; Ambiguous **[ ]**
Classification: Sensitizing **[ ]**; Not sensitizing **[x]**
Method: OECD Guideline No. 406 referenced as Method B6 in Commision Directive 84/449/EEC (which consitutes Annex V of Council Directive 67/548/EEC)
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: Naugalube® 640, purity: 99%
Remarks:
Reference: Safepharm Laboratories, Inc./ Uniroyal Chemical Company, Inc. sponsor. ..

*5.4 REPEATED DOSE TOXICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Post exposure observation period:
Dose:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL:
LOEL:
Results:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Reference:

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type:
System of testing:
Concentration:
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:

Without metabolic activation:
Precipitation conc:
Genotoxic effects: + ? -
With metabolic activation: [ ] [ ] [ ]
Without metabolic activation: [ ] [ ] [ ]
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

B. NON-BACTERIAL IN VITRO TEST

Type:
System of testing:
Concentration:
Metabolic activation: With [ ]; Without [ ]; With and Without [ ]; No data [ ]
Results:
Cytotoxicity conc: With metabolic activation:
Without metabolic activation:
Precipitation conc:
Genotoxic effects: + ? -
With metabolic activation: [ ] [ ] [ ]
Without metabolic activation: [ ] [ ] [ ]
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

*** 5.6 GENETIC TOXICITY IN VIVO**

Type:
Species/strain:
Sex: Female [ ]; Male [ ]; Male/Female [ ]; No data [ ]
Route of Administration:
Exposure period:
Doses:
Results:
Effect on mitotic
index or P/N ratio:
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

5.7 CARCINOGENICITY

Species/strain:
Sex: Female [ ]; Male [ ]; Male/Female [ ]; No data [ ]
Route of Administration:

Exposure period:
Frequency of treatment:
Postexposure observation period:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**;
Other **[ ]**
Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Post exposure observation period:
Premating exposure period: male: . . . . . , female: .....
Duration of the test:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Parental:
NOEL F1 Offspring:
NOEL F2 Offspring:
Results:
General parental toxicity:
Toxicity to offspring:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration: .
Duration of the test:
Exposure period:
Frequency of treatment:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity:
NOEL teratogenicity :
Results:

Maternal general toxicity:
Pregnancy/litter data:
Foetal data:

Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: purity:
Remarks:
Reference:

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type:
Results:
Remarks:
Reference:

B. Toxicodynamics, toxicokinetics

Type:
Results:
Remarks:
References:

I U C L I D

D a t a S e t

New Chemical	Substance ID: 68442-68-2
CAS No.	68442-68-2
EINECS No.	270-485-3
EINECS Name	Benzenamine, N-phenyl-, styrenated
CAS Name	Benzenamine, N-phenyl-, styrenated

Type: Lead organization
Name: American Chemistry Council (formerly Chemical Manufacturers Association) Rubber and Plastics Additives (RAPA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States
Phone: 703-741-5600
Facsimile: 703-741-6091

Type: cooperating company
Name: Bayer Polymers LLC
Country: United States

Type: cooperating company
Name: Ciba Specialty Chemicals Corporation
Country: United States

Type: cooperating company
Name: Crompton Corporation
Country: United States

Type: cooperating company
Name: Flexsys America L.P.
Country: United States

Type: cooperating company
Name: Noveon, Inc (formerly BF Goodrich)
Country: United States

Type: cooperating company
Name: R.T. Vanderbilt Company, Inc.
Country: United States

Type: cooperating company
Name: The Goodyear Tire & Rubber Company
Country: United States

Type: cooperating company
Name: Eliokem Inc.
Country: United States

Type: cooperating company
Name: The Lubrizol Corporation
Country: United States

Type: cooperating company
Name: UOP, LLC.
Country: United States

Number of Pages: 15

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential

Printing date: 25-Feb-03
Revision date:
Date of last Update: 25-Feb-03

1.1 General Substance Information

Substance type: organic
Physical status: liquid
Purity: > 98 % w/w
Result: Molecular weight: 320
25-Feb-03

1.2 Synonyms

Mixed styrenated diphenylamines

N-Phenyl benzenamine, styrenated

p-Oriented styrenated diphenylamines

Styrene, reaction product with diphenylamine

SDPA

Styrenated diphenylamine

Styrenated N-phenylbenzenamine

Vulkanox DDA

WINGSTAY 29

WINGSTAY 29 POWDERED

WINGSTAY 29E

WTR Number 8b

1.3 Impurities

CAS-No: 122-39-4
EINECS-No: 204-539-4
CAS Name: Benzenamine, N-phenyl-
EINECS-Name: diphenylamine
Contents: < .5 % w/w

1.4 Additives

CAS-No: 63231-67-1
CAS Name: Silica gel
EINECS-Name: Siica, hydrated amorphous
Contents: 30 % w/w
Remark: It is also sold as a powder that consists of 70% styrenated diphenylamine and 30% inert carrier. (7)

2.1 Melting Point

Value: ca. 6 degree C
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Remark: Solidifying point
Reliability: (4) not assignable

(8)

2.2 Boiling Point

Value: > 300 degree C at 1013 hPa
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Remark: Actual method is unknown
Reliability: (4) not assignable

(8)

2.3 Density

Type: density
Value: ca. 1.1 g/cm3 at 20 degree C
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable

(8)

Type:
Value:
Method: other: ASTM D-891
Year: 1994
GLP: no data
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Specific Gravity is 1.08-1.10
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(12)

2.4 Vapour Pressure

Value: < 100 hPa at 50 degree C
Method: other (measured)
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable

(8)

2.5 Partition Coefficient

log Pow: 4.64 at 22 degree C
Method: other (measured)
Year: 1990
GLP: yes
Test substance: Vulkanox DDA
Reliability: (1) valid without restriction

(1)

2.6.1 Water Solubility

Value: .41 mg/l at 20 degree C
Qualitative: of very low solubility
Method: Directive 84/449/EEC, A.6 "Water solubility"
Year: 1990
GLP: yes
Test substance: Vulkanox DDA
Reliability: (1) valid without restriction

(1)

2.7 Flash Point

Value: > 100 degree C
Type: open cup
Method: other
Year: 1994
GLP: no data
Remark: Actual method is unknown

Value: 270 degree C
Type:
Method: other
Year: 1994
GLP: no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable

(8)

3.5 Biodegradation

Type: anaerobic
Inoculum: predominantly domestic sewage
Concentration: 100 mg/l related to Test substance
Degradation: 9 % after 28 day
Method: other: OECD Guideline 30 C, modified according to EEC Round-robin-test "Assessment of Biodegradability of Chemicals in Water by Manometric Respiratory DGX 1/283/82 Rec. 5 EEC Directive 79/831 Annex V Part C"
Year: 1986 **GLP:** no
Test substance: Vulkanox DDA
Test substance: Batch No. C 40021 f 28.09.86
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(1)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other
Method: other
Test substance: Vulkanox DDA
Remark: ThOD: 2882 mg/g
Reliability: (4) not assignable

(1)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: 422
LC50: 920
LC100: 2400
Method: other
Year: 1986 **GLP:** no
Remark: Test substance dispersed in water by means of an Ultra-Turrax
Test substance: Vulkanox DDA
Test substance: Batch No. C 40021 of 28.08.86
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(1)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: > 10000
Method: ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year: 1986 **GLP:** no
Remark: Direct weight
Test substance: Vulkanox DDA
Test substance: Batch No. C 40021 of 28.09.86
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(1)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex: no data
Number of Animals: 25
Vehicle: other: corn oil
Value: > 20000 mg/kg bw
Method: other
Year: 1976 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

Remark: The material was placed in a 25% corn oil solution and administered at dosages of 2500, 5000, 10000, 20000, and 40000 mg/kg to five rats each. The animals were observed for 14 days. Two of the five animals died at the dosages of 20000 and 40000 mg/kg.
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.
(5)

Type: LD50
Species: rat
Sex: male/female
Number of Animals: 10
Vehicle: other: corn oil
Value: > 500 mg/kg bw
Method: other: United States Department of Transportation Regulations, 49CFR173.132(1992)
Year: 1993 **GLP:** yes
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Method: Five (5) male and five (5) female young adult rats were administered a single dose of the test substance by gavage. The test substance was dispersed in corn oil at a dosage of 500 mg/kg. The animals were observed for clinical signs of toxicity at approximately 1-, 2.5- and 4-hours following administrations on the day of dosing and daily thereafter for 14-days. Body weights were recorded on Day-minus 1, Day-1, Day-7 and Day-14 of the study. All animals were subjected to a gross necropsy at study termination.
Result: No animals died during the 14-Day observation period. No significant clinical findings and no significant impairment on body weight gains were noted in either the male or female rats. No abnormal tissues were noted in any animals upon necropsy.
Reliability: (1) valid without restriction
(9)

Type: LD50
Species: rat
Sex:
Number of Animals: Unknown
Vehicle:
Value: > 5000 mg/kg bw
Method: other
Year: 1994 **GLP:** no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable

(8)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Sex:
Number of Animals: 5
Vehicle:
Value: > 10000 mg/kg bw
Method: other
Year: 1976 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: No animals died after administration of 10000 mg/kg
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.

(3)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals: Unknown
PDII:
Result: slightly irritating
EC classificat.: not irritating
Method: other
Year: 1976 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Primary Skin Irritation. Was originally classified as non-irritating; however, according to current classifications, it would be a mild irritant. The result was 0.46.
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.

(2)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals: Unknown
PDII:
Result: not irritating
EC classificat.: not irritating
Method: other
Year: 1994 **GLP:** no data
date: 25-Feb-03
Test substance: Vulkanox DDA
Reliability: (4) not assignable
(8)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals: 6
Result: slightly irritating
EC classificat.: not irritating
Method: other
Year: 1976 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Standard protocol of the times for eye irritation. Mild irritant when not followed by wash. Six young adult albino rabbits, three with and three without a wash. Observations were made at 24, 48, and 72 hours and at 7 days.
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure for the time period.
(4)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.: not irritating
Method: other
Year: 1994 **GLP:** no data
Test substance: Vulkanox DDA
Reliability: (4) not assignable
(8)

5.5 Genetic Toxicity 'in Vitro'

Type: Salmonella-Escherichia coli/Mammalian-Microsome Reverse Mutation Assay

System of testing: Salmonella typhimurium (tester strains TA98, TA100, TA1535 and TA1537) and Escherichia coli (tester strain WP2uvrA)

Concentration: 33.3, 100, 333, 1000, 3300, and 5000 ug per plate

Metabolic activation: with and without

Result: negative

Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella typhimurium Reverse Mutation Assay"

Year: 2001 **GLP:** yes

Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)

Method: The objective of the study was to assess the potential of WINGSTAY 29 and/or its metabolites to induce reverse mutations in the presence and absence of a mammalian metabolic activation system with strains of Salmonella typhimurium and Escherichia coli strain WP2uvrA.

Positive controls were 2-nitrofluorene (TA98 without metabolic activation); sodium azide (TA100 and TA1535 without metabolic activation); IRC-191 (TA1537 without metabolic activation); 4-nitroquinoline-N-oxide (WP2uvrA without metabolic activation); benzo[a]byrene (TA98 with metabolic activation); and 2-Aminoanthracene (TA100, TA1535, TA1537, and WP2uvrA with metabolic activation).

Based on results of a range-finding study with Salmonella typhimurium (tester starin TA100) and Escherichia coli (tester strain WP2uvrA), the doses for the test were 33.3, 100, 333, 1000, 3300 and 5000 ug per plate of WINGSTAY 29 in both the presence and absence of S9 metabolic activation. The assay used plate incorporation methodology. S. typhimurium strains TA98, TA100, TA1535 and TA1537, and the E. coli strain WP2uvrA were used. Following incubation, revertant colonies (mutations) were counted. The exogenous metabolic activation system was derived from Aroclor-induced Sprague-Dawley rat livers (S9). Dimethylsulfoxide (DMSO) was used as the vehicle for WINGSTAY 29. Vehicle and positive controls were included in the assay. All doses of WINGSTAY 29, the vehicle control, and positive controls were plated in triplicate.

The results of the initial assay were confirmed in an independent test.

No increase in the number of revertant colonies was seen in plates dosed with WINGSTAY 29 in the presence or absence of S9 metabolic activation in the initial and confirmatory assays. All criteria for acceptable assays were met.

Result: WINGSTAY 29 did not cause reverse mutations in the S. typhimurium or E. coli tester strains in the presence or absence of metabolic activation system (rat liver S9).

Reliability: (1) valid without restriction

Type: Ames test
System of testing: Salmonella typhimurium Strains TA-98, 100, 1535, and 1537
Concentration: 1, 10, 100, and 1000 micrograms/l
Metabolic activation: with and without
Result: negative
Method: other
Year: 1980 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Test compound was evaluated for genetic activity in the Ames test with and without the addition of mammalian metabolic activation. Negative and positive controls were run concurrent with the assay. No remark was made regarding which positive control was used with which strain. No remark whether positive controls were duplicate or triplicate.

Positive Controls: without activation - 2-nitrofluorene, sodium azide, quinacrene mustard with activation 2-aminofluorene, 2-aminoanthracene, dimethylbenz(a)anthracene
Negative Control: DMSO
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(13)

Type: Ames test
System of testing: Salmonella typhimurium Strains TA-98, 100, 1535, and 1537
Concentration: 10, 100, and 2000 micrograms/l
Metabolic activation: with and without
Result: negative
Method: other
Year: 1982 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Remark: Test compound was evaluated for genetic activity in the Ames test with and without the addition of mammalian metabolic activation. Negative and positive controls were run concurrent with the assay. No remark was made regarding which positive control was used with which strain. No remark whether positive controls were duplicate or triplicate.

Positive Controls: without activation - 2-nitrofluorene, sodium azide, quinacrene mustard with activation 2-aminofluorene, 2-aminoanthracene, dimethylbenz(a)anthracene
Negative Control: DMSO
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure.

(14)

Type: DNA damage and repair assay
System of testing: Escherichia coli, Strains W 3110 (Pol A+) and p 3478 (Pol A1-)
Concentration: 10, 1000, 2500, and 5000 micrograms/l
Metabolic activation: with and without
Result: negative
Method: other
Year: 1981 **GLP:** no
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Positive Controls: with activation - Tris(2,3 dibromopropyl)phosphate
without activation - Ethyl Methanesulfonate
Negative Control: Chloramphenicol
Remark: A test for the ability of the chemical to damage cellular DNA in the E coli Pol A1- Liquid Suspension Assay. Negative and positive controls were run concurrent with the assay.
Reliability: (2) valid with restrictions
Although this study was probably not conducted to GLP, the test parameters used were based on a known and well established procedure. (11)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse **Sex:** male
Strain: other: Crl:CD-1 (ICR) BR
Route of admin.: gavage
Exposure period: Single oral dose. Harvested 24 and 48 hours after dosing.
Doses: 0, 500, 1000 and 2000 mg/kg
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 2001 **GLP:** yes
Test substance: benzenamine, N-phenol, styrenated (CAS# 68442-68-2)
Method: The objective of the study was to assess the potential of WINGSTAY 29 to induce chromosome damage in vivo in mice. The presence of micronuclei in polychromatic erythrocytes was used as an indicator of clastogenic activity and/or disruption of the mitotic apparatus.

Based on the results of a dose-finding assay, single doses of 0, 500, 1000, and 2000 mg/kg WINGSTAY 29 were administered to male Crl:CD-1 (ICR) BR mice. Corn oil was used as the vehicle. Five male mice per group were evaluated. Bone marrow cells were harvested 24 and 48 hours after dosing. All dose levels, the vehicle control and a positive control (Cyclophosphamide) were evaluated at the 24 hours. At 48 hours, only the vehicle control and high dose were evaluated.

Bone marrow was taken from the hind limbs. Slides were prepared from the bone marrow extracts, fixed with methanol and stained in May Grunwald Solution and Giemsa. Two thousand micronucleated polychromatic erythrocytes were evaluated for micronuclei. The ratio of polychromatic erythrocytes (PCE) to nonchromatic erythrocytes (NCE) cells was determined from the first 500 erythrocytes on each slide.

Statistical analyses were performed using Analysis of Variance and Dunnett's t-test.

Wingstay 29 did not produce any signs of clinical toxicity. Statistically lower PCE:NCE ratios, while not dose related, did strongly indicate that WINGSTAY 29 was cytotoxic to the bone marrow. WINGSTAY 29 did not produce any statistically significant increase in micronucleated PCEs relative to the vehicle control at the 24-hour and 48-hour harvest interval. The positive control induced a statistically significant increase in micronucleated PCEs compared to the vehical control.

Result: Wingstay 29 was tested up to the limit dose (2000 mg/kg) and did not cause chromosome damage in the mouse bone marrow micronucleus assay under the conditions of this test.

Reliability: (1) valid without restriction

(6)

(1) Bayer AG Data

(2) Food and Drug Research Laboratories, Inc., Primary Skin Irritation Study with Rabbits, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976

(3) Food and Drug Research Laboratories, Inc., Acute Dermal Toxicity in Rabbits, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976

(4) Food and Drug Research Laboratories, Inc., Rabbit Eye Irritation Study, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976

(5) Food and Drug Research Laboratories, Inc., The Acute Oral Toxicity in Rats, Laboratory Report No. 2688b to The Goodyear Tire & Rubber Company, 1976.

(6) In Vivo Mouse Micronucleus Assay with WINGSTAY 29, Reprt #; 21054-0-455OECD, Covance Laboratories (Vienna, Virginia), 1/19/01

(7) It is also sold as a powder that consists of 70% styrenated diphenylamine and 30 % inert carrier.

(8) Material Safety Data Sheet, Bayer AG, 1994

(9) Ricerca Inc., Study No. 5797-93-0196-TX-000 to The Goodyear Tire & Rubber Company, 1993

(10) Salmonella-Escherichia coli/Mammalian-Microsome Reverse Mutation Assay with a Confirmatory Assay with WINGSTAY 29, Report #: 21054-0-409OECD, Covance Laboratories (Vienna, Virginia), 02/06/01

(11) The Goodyear Tire & Rubber Company, E. coli Pol A1- Liquid Suspension Assay on WINGSTAY 29, 1981.

(12) The Goodyear Tire & Rubber Company, Material Safety Data Sheet, 1994

(13) The Goodyear Tire & Rubber Company, Mutagenicity Evaluation of WINGSTAY 29, 1980.

(14) The Goodyear Tire & Rubber Company, Mutagenicity Evaluation of WINGSTAY 29, Laboratory Report No. 82-1-1, 1982.

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, N-phenyl-, reaction products with isobutylene and 2, 4, 4-trimethylpentene

CAS No. 184378-08-3

Sponsor Country : . . . . . .

DATE: . . . . . .

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 184378-08-3

B. Name *(IUPAC name)*

***C. Name** *(OECD name)*

†D. CAS Descriptor Benzenamine, N-phenyl-, reaction products with isobutylene and 2, 4, 4-trimethylpentene

E. EINECS-Number 270-128-1

F. Molecular Formula

***G. Structural Formula**

H. Substance Group

I. Substance Remark

J. Molecular Weight 225-393

1.02 OECD INFORMATION

A. Sponsor Country: United States

B. Lead Organisation:

Name of Lead Organisation: Noveon, Inc.
Contact person: Robert K. Hinderer, Ph.D.
Address:
Street: 9911 Brecksville Rd.
Postal code: 44141-3247
Town: Cleveland, Ohio
Country: U.S.A.
Tel: (216)447-5181
Fax: (216)447-5760

C. Name of responder

Name:
Address:
Street:
Postal code:
Town:
Country:
Tel:
Fax:

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. Purity *(indicate the percentage by weight/weight) 99 %*

1.2 SYNONYMS Good-rite® 3128NT
Vanlube® 961

1.3 IMPURITIES

CAS No: 122-39-4
EINECS No:
Name: Diphenylamine
Value: <1%

Remarks:

1.4 ADDITIVES

CAS No:
EINECS No:
Name:
Value:
Remarks:

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value:	280°K
Decomposition:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	OECD 102
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	The sample was heated in a water bath starting at 19°C. At intervals of 3°C the jar containing the test sample was tilted to a horizontal position for a period of 5 seconds and was observed for signs of flow. The stationary point was determined to be 280°K and the pour point was determined to be 283°K.
Reliability:	(1) Valid without Restrictions
Reference:	O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

MELTING POINT

Value:	44-107°C
Decomposition:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[x]** ? **[ ]**
Remarks:	Range for major components; the melting point for the butylated/octylated component could not be determined because it is an oil.
Reference:	BFGoodrich Laboratory (now Noveon, Inc.)

***2.2 BOILING POINT**

Value:	549 +/- 0.5 K
Pressure:	at 101.02 hPa
Decomposition:	Yes **[X]** No **[ ]** Ambiguous **[ ]**
Method:	OECD 103
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	The boiling point was determined using a Mettler Toledo DSC12E calorimeter under statis air atmosphere. The initial temperature was 20ºC. The temperature was ramped at a rate of 20ºC/min to a final temperature of 400ºC. Because the material decomposed, no value for boiling temperature could be established. Therefore, the boiling temperature was estimated to be in the range of 575 to > 633 K using experimental databases for the diphenylamine impurity and an adaption of the Stein and Brown method (Syracuse Research Corp., Inc. MPBP for Windows version 1.40, William Meylan, (1994-2000) to derive values for individual mono- and di-alkyldiphenylamine components.
Reliability:	(1) Valid without Restrictions
Reference:	O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

BOILING POINT

Value:	>200 °C
Pressure:	at . . . . . hPa
Decomposition:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:	
Reference:	Noveon, Inc. MSDS

BOILING POINT

Value:	Approx. 370 °C
Pressure:	at . . . . . hPa
Decomposition:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	EPIWIN
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:	326.04 to 431.62 for major components
Reference:	EPIWIN

†2.3 DENSITY (relative density)

Type:	Bulk density **[ ]**; Density **[X]**; Relative Density **[ ] Specific Gravity**
Value:	977 kg/m^3
Temperature:	20.0 +/- 0.5 °C
Method:	OECD 109, 27 July 1995
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	A calibration was carried out by determing the mass of distilled water required to fill the glass pycnometer. The mass of the test material required to fill the pycnometer then was determined.
Reliability:	(1) Valid without Restrictions
Reference:	O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

DENSITY (relative density)

Type:	Bulk density **[ ]**; Density **[ ]**; Relative Density **[ ] Specific Gravity**
Value:	Approx. 1
Temperature:	°C
Method:	Unknown
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	
Reference:	Noveon, Inc. MSDS

*2.4 VAPOUR PRESSURE

Value:	$9.4x10^{-5}$ Pa
Temperature:	25. . . . . °C
Method:	calculated **[ ]**; measured **[ ]** OECD 104
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	The vapour pressure was determined using a vapour pressure balance with a sensitivity of approximately 0.1 µg. Temperature of the sample was controlled automatically and the temperature and mass readings were recorded automatically.
Reliability:	(1) Valid without Restrictions
Reference:	Tremain, S.P. (2002). Vanlube 961: Determination of Vapour Pressure, SafePharm Laboratories, Ltd.

VAPOUR PRESSURE

Value:	2x10-5 mmHg hPa
Temperature:	25°C
Method:	calculated **[ ]**; measured **[ ]** Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[x]**
Remarks:	CAS# 68411-46-1 has similar reaction products as CAS# 184378-08-3. Uniroyal MSDS for CAS#68411-46-1 indicates negligible @20 degrees C .
Reference:	CIBA MSDS for CAS# 68411-46-1

VAPOUR PRESSURE

Value: 1.14E-004 to 5.05E-008 hPa
Temperature: °C
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Range for major components
Reference: EPIWIN

***2.5 PARTITION COEFFICIENT $log_{10}P_{ow}$**

Log Pow: $1.34x10^4$ to > $1.59x10^6$, log_{10} P_{ow} 3.13 to >6.20
Temperature: . °C
Method: calculated **[ ]**; measured **[X]** OECD 117
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Remarks: Following a preliminary test to approximate the solubilities of the test material in n-octanol and water, the test material (0.0276g) was diluted to 100 ml with acetonitrile. Solutions of reference standards also were prepared. The sample, thiourea, and referenced standard solutions were injected in duplicate in an HPLC , calibration curves were constructed, and retention times were determined. The capacity factors and log_{10} P_{ow} values then were calculated.
Reliability: (1) Valid without Restrictions
Reference: O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

PARTITION COEFFICIENT $log_{10}P_{ow}$

Log Pow: >>6
Temperature: °C
Method: calculated **[ ]**; measured **[ ]** Unknown
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: CAS# 68411-46-1 has similar reaction products as CAS# 184378-08-3.
Reference: CIBA MSDS for CAS# 68411-46-1

PARTITION COEFFICIENT $log_{10}P_{ow}$

Log Pow: 5.2 to 10.82
Temperature: °C
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Range for major components
Reference: EPIWIN

***2.6 WATER SOLUBILITY**

Value: $9.09\ x10^{-2}$ to $5.93x10^{-5}$
Temperature: 20.0 +/- 0.5°C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[X]**; Not soluble **[ ]**
Method: OECD 105
GLP: Yes **[X]** No **[ ]** ? **[ ]**

Remarks:	An aliquote (0.5744g) of the test material was diluted to 500 ml with glass double distilled water. After shaking for 3¼ hours at 30°C and standing four 18 hours at 20°C, the solution was analysed by HPLC. The concentrations of the individual mono- and di-alkyldiphenylamine components and diphenylamine impurity ranged from 9.09 $x10^{-2}$ (DPA) to $5.93x10^{-5}$. These values are the means of three samples.
Reliability:	(1) Valid without Restrictions
Reference:	O'Connor, B.J. and Mullee, D.M. (2002). Vanlube 961: Determination of General Physico-chemical Properties, SafePharm Laboratories, Ltd.

WATER SOLUBILITY

Value:	<0.01%
Temperature:	°C
Description:	Miscible **[ ]**; Of very high solubility **[ ]**; Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**; Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:	CAS# 68411-46-1 has similar reaction products as CAS# 184378-08-3.
Reference:	CIBA MSDS. for CAS# 68411-46-1

WATER SOLUBILITY

Value:	1.167 to 1.939e-006 mg/l
Temperature:	°C
Description:	Miscible **[ ]**; Of very high solubility **[ ]**; Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**; Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:	EPIWIN
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:	
Reference:	EPIWIN

2.7 FLASH POINT

Value:	>180 °C
Type of test:	Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method:	Pensky Martens.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	
Reference:	BFGoodrich MSDS (Flash range)

2.8 AUTO FLAMMABILITY

Value:	°C
Pressure:	hPa
Method:	
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:	
Reference:	

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;
More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

†2.12 OXIDATION: REDUCTION POTENTIAL

Value: mV
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]** Remarks:
Reference:

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

B. Other data

Results:
Remarks:
Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: nm
Relative intensity:
Spectrum of substance: nm
Concentration of Substance:
Temperature: °C
Direct photolysis:
Half life: 0.053 days
Degradation: % (weight/weight) after (exposure time)
Quantum yield:
Indirect Photolysis:
Type of sensitizer:
Concentration of sensitizer:
Rate constant (radical): cm^3/molecule*sec
Degradation:
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference: EPIWIN

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: at pH at °C
Degradation: at pH at °C after
(exposure time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration:
Soil temperature: °C
Soil humidity:
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year
Content of clay etc.: Clay %, Silt %, Sand %
Organic Carbon:
Soil pH:
Cation exchange capacity:
Microbial biomass:
Dissipation time: DT 50 :
DT 90 :
Dissipation : % after (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

*3.2 MONITORING DATA (ENVIRONMENTAL)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media:
Results:
Remarks:
Reference:

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media:
Method:
Results:
Remarks:
Reference:

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPOIWIN. .....
Results: Air 0.0697% to 0.0105%; 1.28hr to 1.26 hr half-life; 1000 kg/hr
Water 17.4% to 1.27%; 900 hr to 3.6e+003 half-life; 1000 kg/hr

Soil 49.6% to 32 %, 900 hr to 3.6e+003 half-life, 1000 kg/hr
Sediment 33% to 66.7%, 3.6e+003 to 1.44e+004 half-life, 0 kg/hr. .....

Remarks:
Reference: EPIWIN

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results:
Remarks:
Reference:

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ]**; water-sediment **[ ]**; soil **[ ]**; sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
% after (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ]**; inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) % in (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5
Method:
Concentration: related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: mg O_2/l
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method:
Value: mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD_5/COD:
Remarks:
Reference:

3.7 BIOACCUMULATION

Species:
Exposure period:
Temperature: °C
Concentration
BCF:
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**

Method:
Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Reference:

3.8 ADDITIONAL REMARKS

A. Sewage treatment

Results:
Remarks:
Reference:

B. Other information

Results:
Remarks:
Reference:

4. <u>ECOTOXICITY</u>

***4.1 ACUTE/PROLONGED TOXICITY TO FISH**

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: LC_{50} (24h) = mg/l
LC_{50} (48h) = mg/l
LC_{50} (72h) = mg/l
LC_{50} (96h) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

***A. Daphnia**

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**;
open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: EC_{50} (24h) = mg/l
EC_{50} (48h) = mg/l
EC_{xx} (..h) = mg/l

NOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: EC_{50} (24h) = mg/l
EC_{50} (48h) = mg/l
EC_{xx} (..h) = mg/l
NOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

***4.3 TOXICITY TO AQUATIC PLANTS**

Species:
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (h) = mg/l
(Endpoint) EC_{xx} (h) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.4 TOXICITY TO BACTERIA

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:
Exposure Period:
Results: EC_{50} (. . . h) = mg/l
EC_{xx} (. . . h) = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:

Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**
Exposure period:
Results: . EC_{50} (..d) = mg/l
(Endpoint) EC_{xx} (..d) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (. . . . . h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**

Species:
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (. . . . . d) = ... mg/kg
(Endpoint) EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

(b)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:
(c)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l

LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: ....., purity: .....
Remarks:
Reference:

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

Results: Substance:
Species or ecosystem studied:
Effects monitored:
Results:
Chemical analysis:
Remarks: *(Information on environmental conditions (e.g. water characteristics: suspended matter, pH, temperature, hardness; soil/sediment characteristics: % organic matter, clay content)*

Reference:

4.8 BIOTRANSFORMATION AND KINETICS

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results:
Remarks:
Reference:

4.9 ADDITIONAL REMARKS

Results:
Remarks:
Reference:

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: Sprague-Dawley CD rats
Value: >2500 mg/kg b.w.:
Discriminating dose:
Method: OECD 423
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Vanlube 961 purity: 99%
Remarks: The test material was administered by a single gavage dose as a solution in arachis oil. A group of three fasted females was treated with the test material at a dose of 2000 mg/kg b.w. After allowing a sufficient time to determine survival in the female, a group of three fasted males then was treated with the test material at a dose of 2000 mg/kg b.w. Animals were observed for deaths or signs of toxicity at ½, 1, 2, and 4 hours after dosing and then once daily for fourteen days. Body weights were determined prior to dosing and at seven and fourteen days post exposure. All animals were subject to a gross pathological examination at termination. No deaths, signs of toxicity, or abnormalities were observed. Body weight gains were normal. Based on the test procedure the LD_{50} was estimated to be greater than 2500 mg/kg b.w.
Reliability: (1) Valid without Restrictions
Reference: Driscoll, R. (2002). Vanlube 961: Acute Oral Toxicity in the Rat – Acute Toxic Class Method, SafePharm Laboratories, Ltd.

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
Species/strain:
Exposure time:
Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Value: mg/kg b.w.
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Route of Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time:
Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain:
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification:
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.2.2 EYE IRRITATION/CORROSION

Species/strain:
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification:
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.3 SKIN SENSITISATION

Type: Magnusson & Kligman Maximazation Test
Species/strain: Guinea Pig/Dunkin Hartley
Results: Sensitizing **[ ]**; Not sensitizing **[x]**; Ambiguous **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Sensitizing **[ ]**; Not sensitizing **[x]**
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

OECD 406 B6 of EC Directive 92/69/EEC .....

GLP: Yes **[x]** No **[ ]** ? **[ ]**

Test substance: Good-rite® 3128 (Vanlube® 961) , purity: 99%

Remarks: Twenty test and ten control animals were used in this study. Based on the results of the sighting tests, the concentrations of the test material was selected as follows:

Intradermal induction – A row of three injections (0.1 ml each): a)Freund's Complete Adjuvant/ water (1:1), b)25% in arachis oil BP, and c) 25% in arachis oil BP in a 1:1 preparation of Freund's Complete Adjuvant in water; sites were evaluated at 24 and 48 hrs. Control animals received a)Freund's Complete Adjuvant/ water (1:1), b)arachis oil BP, and c) a 50% formulation of arachis oil BP in Freund's Complete Adjuvant/ water 1:1 and evaluated as the same as the test material.

Topical induction –7days after the injections undiluted as supplied was applied to the same area on the clipped shoulder region and covered by an occlusive patch. After 48 hrs the patch was removed and the site was evaluated.

Topical Challenge – On Day 21 undiluted as supplied and 75% in arachis oil BP was applied to a clipped area and covered with an occlusive patch. After 24 hrs the patch was removed; skin reactions were evaluated at 24 and 48 hours.

The intradermal and topical induction doses were based on the highest concentration that caused only mild to moderate irritation and was well tolerated systemically. The highest non-irritating concentration and one lower concentration were selected for the topical challenge.

The test material produced 0% (0/20) sensitization rate and was classified as a non-sensitizer to the guinea pig skin.

Reliability: (1) Valid without Restrictions

. Reference: Safepharm Laboratories Limited, 1996

*5.4 REPEATED DOSE TOXICITY

Species/strain:

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Route of Administration:

Exposure period:

Frequency of treatment:

Post exposure observation period:

Dose:

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL:

LOEL:

Results:

Method:

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Test substance: . . . . . , purity: . . . . . .

Reference:

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: Bacterial reverse mutation assay
System of testing: *Salmonella typhimurium* strains TA1535, TA1537, TA102, TA98, TA100
Concentration: 0, 50, 150, 500, 1500, 5000 µg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: None at concentrations tested.
Without metabolic activation: None at concentrations tested.
Precipitation conc: None observed.
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[X]**
Without metabolic activation:	**[ ]**	**[ ]**	**[X]**

Method: OECD 471
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Vanlube 961, purity: 99%
Remarks: The strains were obtained from the University of California. Overnight sub-cultures were prepared in nutrient broth and incubated at 37°C fo approximately 10 hours. The test material was dissolved in DMSO. Vehicle and positive controls were tested in parallel with the test material. A solvent treat ment group was the vehicle control and the positive controls were as follows: **without liver S-9 activation** N-ethyle-N'-nitro-N-nitrosoguanidine (3µg/plate for TA100; 5µg/plate for TA1535), 9-aminoacridine (80µg/plate for TA1537), Mitomycin C (0.5µg/plate for TA102), 4-nitroquinoline (0.2µg/plate for TA198) and **with liver S-9 activation** 2-aminoanthracene (1µg/plate for TA100, 2µg/plate for TA11535 and TA1537), Benzo(a)pyrene (5µg/plate for TA98), 1,8-dihydroxyanthraquinone (10µg/plate for TA102).

Based on the preliminary toxicity studies a first experiment was conducted. The test material was assayed in triplicate using the concentrations described above. The test material formulation (0.l ml) was added to the agar plates with and without S-9. All plates were incubated at 37ºC for 48 hours and then the frequency of revertant colonies was assessed. A second experiment was then conducted in the same manner as the first.

The assay was considered valid if all spontaneous revertants were in normal ranges, all tester strain characheristics were confirmed and all tester strain cultures were in the approximate range of 1 to $9.9x10^9$ bacteria per ml.

The test material was considered positive if it induced a reproducible, dose-related and statistically significant increase in the revertant count in at least one strain of bacteria.

In both experiments the revertant counts at all concentrations for all strains, both with and without S-9, were comparable to the vehicle control. Also, all positive controls performed normally. Based on the absence of any significant increases in the frequency of revertant colonies, the test material was considered to be non-mutagenic under the conditions of the test.

Reliability: (1) Valid without Restrictions
Reference: Thompson, P.W. (2002). Vanlube 961: Reverse Mutation Assay "Ames Test" Using *Salmonella typhimurium*, SafePharm Laboratories, Ltd.

B. NON-BACTERIAL IN VITRO TEST

Type:
System of testing:
Concentration:
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:.
Without metabolic activation:
Precipitation conc:
Genotoxic effects: + ? -
With metabolic activation: **[ ] [ ] [ ]**
Without metabolic activation: **[ ] [ ] [ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*** 5.6 GENETIC TOXICITY IN VIVO**

Type:
Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Doses:
Results:
Effect on mitotic index or P/N ratio:
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.7 CARCINOGENICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Postexposure observation period:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

Results:
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility [ ]; One-generation study [ ]; Two-generation study [ ]; Other [ ]
Species/strain:
Sex: Female [ ]; Male [ ]; Male/Female [ ]; No data [ ]
Route of Administration:
Exposure period:
Frequency of treatment:
Post exposure observation period:
Premating exposure period: male: . . . . . , female: .....
Duration of the test:
Doses:
Control group: Yes [ ]; No [ ]; No data [ ];
Concurrent no treatment [ ]; Concurrent vehicle [ ]; Historical [ ]
NOEL Parental:
NOEL F1 Offspring:
NOEL F2 Offspring:
Results:
General parental toxicity: .....
Toxicity to offspring:
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain:
Sex: Female [ ]; Male [ ]; Male/Female [ ]; No data [ ]
Route of Administration:
Duration of the test:
Exposure period:
Frequency of treatment:
Doses:
Control group: Yes [ ]; No [ ]; No data [ ];
Concurrent no treatment [ ]; Concurrent vehicle [ ]; Historical [ ]
NOEL Maternal Toxicity:
NOEL teratogenicity :
Results:
Maternal general toxicity:
Pregnancy/litter data:
Foetal data:
Method:
GLP: Yes [ ] No [ ] ? [ ]

Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: *(e.g. neurotoxicity, immunotoxicity, etc.)*

Results:
Remarks:
Reference:

B. Toxicodynamics, toxicokinetics

Type:

Results:
Remarks:
References:

I U C L I D

Data Set

Existing Chemical	:	ID: 10081-67-1
CAS No.	:	10081-67-1
EINECS Name	:	4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline
EC No.	:	233-215-5
Molecular Formula	:	C30H31N

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	14.07.2003

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	14.07.2003
Status	:	
Memo	:	RAPA
Printing date	:	14.07.2003
Revision date	:	
Date of last update	:	14.07.2003
Number of pages	:	15
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	
Physical status	:	solid
Purity	:	
Colour	:	white to off-white
Odour	:	characteristic

14.07.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

14.07.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 98.5 °C
Sublimation	:	
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	98.5 deg C at STP
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions

14.07.2003 (1)

2.2 BOILING POINT

2.3 DENSITY

Type	:	density
Value	:	= 1.14 g/cm³ at °C
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions

14.07.2003 (1)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

2.5 PARTITION COEFFICIENT

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	2003
GLP	:	no data

Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Insoluble
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
14.07.2003		(1)
Solubility in	:	Organic Solvents
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Soluble
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
14.07.2003		(1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 276.7 °C
Type	:	
Method	:	other: Tag Closed Cup
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
14.07.2003		(1)

2.8 AUTO FLAMMABILITY

Value	:	= 298 - °C at
Method	:	
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
14.07.2003		(1)

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Crompton Material Safety Data Sheet (2003) Naugard 445. Revision 1.1 05/28/2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

101-67-7
Benzenamine, 4-octyl-N-(octylphenyl)-

Molecular Formula: **C28-H43-N**
Molecular Weight: **393.72**

1.1 GENERAL SUBSTANCE INFORMATION

A.	**Type of Substance:**	Organic
B.	**Physical State:**	Tan Solid
C.	**Purity:**	90-95 % Typical for Commercial Products

1.2 SYNONYMS

ODPA
Octylated Diphenylamine
Flectol® ODP
Vulcanox OCD
Permanax® ODPA
Octamine®

1.3 IMPURITIES

Mono-octylated amine (CAS# 4175-37-5) 5-10%
Tri-octylated amine <5%

1.4 ADDITIVES

None

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value:	87-95°C
Decomposition:	No
Sublimation:	No
Method:	FF83.9-1 Initial and Final Melt Point of Organic Compounds
: GLP:	Yes
Remarks:	Capillary Melt Point
Reference:	ASTM D-1519 / Flexsys Standard Physical Methods of Analysis
Reliability:	(1) Valid without restriction

*2.2 BOILING POINT

Value:	200°C
Pressure:	0.66661 hPa
Decomposition:	No data
Method:	Not Specified
GLP:	No data
Remarks:	None
Reference:	Monsanto Company MSDS Flectol ODP May 1971
Reliability:	(2) Valid with restrictions – lack of method detail

†2.3 DENSITY (relative density)

Type:	Density
Value:	1.015

Temperature:	20 °C
Method:	FF97.8-1 Flexsys Standard Method 1997
GLP:	Yes
Remarks:	Density of solids by displacement
Reference:	Flexsys Standard Physical Methods of Analysis
Reliability:	(1) Valid without restriction

***2.4 VAPOUR PRESSURE**

Value:	<0.13332 hPa
Temperature:	Not Specified
Method:	No data
GLP:	No data
Remarks:	None
Reference:	Monsanto Company MSDS Flectol ODP May 1971
Reliability:	(2) Valid with restrictions – no method details

***2.5 PARTITION COEFFICIENT $log_{10}P_{ow}$**

Log Pow:	11.26
Temperature:	Not Applicable
Method:	calculated SRC LogKow (KowWin) Program, 1995.
GLP:	No
Remarks:	Estimation method based on molecular structure
Reference:	EPIWIN/KOWWIN v1.66
Reliability:	(2) Valid with restrictions – modelling data

.

***2.6 WATER SOLUBILITY**

A. Solubility

Value:	<0.1g/100 ml
Temperature:	21°C
Description:	Of very low solubility
Method:	Not Specified
GLP:	No data
Remarks:	None
Reference:	Hawley,G.G. The Condensed Chemical Dictionary, 1977.313
Reliability:	(4) Not assignable - data from a secondary literature source

Value:	4.215e-007
Temperature:	25°C
Description:	Of very low solubility
Method:	WSKOW, v1.40
GLP:	No
Remarks:	Estimation method based on molecular structure
Reference:	EPIWIN/WSKOW v1.40
Reliability:	(2) Valid with restrictions – modelling data

B. pH Value, pKa Value

2.11 OXIDISING PROPERTIES

†2.12 OXIDATION: REDUCTION POTENTIAL

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

B. Other data – Henry's Law Constant

Results:	6.76E-005 atm-m3 /mole
Remarks:	Calculated value from moist soil surfaces @ 25°C
Reference:	Environ Toxicol Chem 10: 1283-93 (1991) EPIWIN/HENRYWIN v3.10
Reliability:	(2) Valid with restrictions – modelling data

3. <u>ENVIRONMENTAL FATE AND PATHWAYS</u>

***3.1.1 PHOTODEGRADATION**

Type:	Air
Light source:	Sunlight
Temperature:	25°C
Direct photolysis:	
Half life:	0.049 Days; 0.586 Hours
Indirect Photolysis:	
Rate constant (radical):	219.0603 E-12 cm^3/molecule-sec
Method:	calculated Atmospheric Oxidation Program/SAR Methods, 1995
GLP:	No
Test substance:	Other: SAR
Remarks:	Rapid atmospheric degradation of test substance in vapor phase by reaction with photochemically produced hydroxyl radicals.
Reference:	Meylan, WH and Howard, PH, Chemosphere 26: 1193-99, 1999 EPIWIN/AOPWIN v1.90
Reliability:	(2) Valid with restrictions – modelling data

***3.1.2 STABILITY IN WATER**

***3.2 MONITORING DATA (ENVIRONMENTAL)**

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

***3.3.1 TRANSPORT**

Type:	Adsorption
Media:	Soil/Sediment
Method:	SRC Structure estimation method based on molecular connectivity indices, 1992
Results:	Koc = 2.864E+007 Log Koc = 7.457
Remarks:	The Koc value suggests that the test substance will have a very high mobility in soil and will tend to adsorb to suspended solids and sediment in water.

Reference: EPIWIN/PCKOCWIN v1.66
Reliability: (2) Valid with restrictions – modelling data

Type: Volatility
Media: Water
Method: Estimation Method, 1990
Results: Volatilization half-life from model river: 2.027 Hours
Volatilization half-life from model lake: 188.5 Hours (7.853 Days)
Volatilization from water: 0.518 atm-m3/mole
Remarks: Model river = 1 m deep flowing at 1 m/sec and wind velocity of 3 m/sec.
Model lake = 1 m deep flowing at 0.05 m/sec and wind velocity of 0.5 m/sec.
Reference: Handbook of Chemical Property Estimation Methods, 1990
Reliability: (2) Valid with restrictions – modelling data

***3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)**

Media: Air-biota-sediment-soil-water
Method: Fugacity level III
EPIWIN v3.10
Results:

	Mass Amount (%)	Half-life (hrs)	Emissions (kg/hr)
Air	0.0348	1.17	1000
Water	3.49	900.00	1000
Soil	27.1	900.00	1000
Sediment	69.3	3.6e+003	0

Remarks: Persistence time estimated at 1.59e+003 Hours
Reference: EPISUITE/EPIWIN v3.10
Reliability: (2) Valid with restrictions – modelling data

***3.5 BIODEGRADATION**

Media: Wastewater Treatment
Method: BIOWIN v4.00
Results: Removal in Wastewater Treatment
Total Removal: 94.04%
Total Biodegradation: 0.78%
Total Sludge Adsorption: 93.25%
Total to Air: 0.00%
Reference: EPISUITE/EPIWIN v3.10
Reliability: (2) Valid with restrictions – modelling data

3.6 BIOACCUMULATION

Species: None
Exposure Period: Not Applicable
Temperature: Not Applicable
Concentration: Not Applicable
BCF: 3.162
Elimination: No
Method: BCFWIN v2.14

Type of test:	Calculated
	Other
GLP:	No
Test substance:	As specified in 1.1-1.4
Remarks:	Calculated using a Log P of 11.26
Reference:	EPIWIN/BCFWIN v2.14
Reliability:	(2) Valid with restrictions – modelling data

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test:	static
	Closed system
Species:	Bluegill Sunfish (lepomis machrochirus)
Exposure period:	96 hours
Results:	LC_{50} (24h) = >1000 mg/l
	LC_{50} (48h) = >1000 mg/l
	LC_{50} (72h) = >1000 mg/l
	LC_{50} (96h) = >1000 mg/l
	NOEC = 1000 mg/l
	LOEC = Not determined
Analytical monitoring:	No
Method:	Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians.
	EPA Ecological Research Series EPA-660/3-75-009 April 1975
GLP:	Yes
Test substance:	As prescribed by 1.1-1.4, purity: >90%
Remarks:	Test fish were obtained from Osage Catfisheries in Osage Beach, Missouri. Test fish were held in culture tanks on a 16-hour daylight photoperiod and observed for at least 14 days prior to testing. A daily record of fish observations was maintained during the holding period, during which time the fish were fed a standard diet of commercial fish food until 48 hours prior to testing, when feeding was stopped. A 96-hour range-finding test preceded the definitive study. Test fish had a mean weight of 0.17 g and a mean standard length of 20 mm. The test was conducted in 5-gallon glass vessels containing 15 liters of laboratory well water. The 0-hour measured control water parameters of this dilution water were dissolved oxygen 8.5 mg/l and pH 7.8. The test vessels were kept in a water bath at 22°C. Test fish were acclimated to the dilution water and test temperature, and held without food for 48 hours prior to testing. Nanograde Acetone was used to prepare the test solutions and as the solvent control. Ten fish per concentration were placed in the testing vessels within 20 minutes of the addition of the test material aliquots. The compound was tested over a range from 100 to 1000 mg/ml. All concentrations were observed once every 24 hours for mortality and abnormal effects. Dissolved oxygen values and pH ranges were monitored during the testing and remained within acceptable limits of 60-97% saturation for dissolved oxygen and pH values of 5.3-8.5. The ammonia concentration was below the toxic limit. Water hardness (CaCO3) was 255 ppm. As a quality check, test fish were challenged with Antimycin A. Statistical analysis of the

	concentration vs. effect data was obtained by employing a computerized program developed by Stephan et al. This program calculated the LC50 statistic and its 95% confidence limits using the binomial, the moving average, and the probit tests. The estimated 96Hr LC50 and 95% confidence limits were within the 95% confidence limits reported in the literature, indicating that the fish were in good condition.
Reference:	Monsanto AB-83-016 Analytical Biochemistry Labs July 1983
Reliability:	(1) Valid without restriction
Type of test:	static Closed system
Species:	Rainbow Trout [Salmo gairdneri]
Exposure period:	96 Hours
Results:	LC_{50} (24h) = >1000 mg/l LC_{50} (48h) = >1000 mg/l LC_{50} (72h) = >1000 mg/l LC_{50} (96h) = >1000 mg/l NOEC = 1000 mg/l LOEC = Not Determined
Analytical monitoring:	No
Method:	Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA Ecological Research Series EPA-660/3-75-009 April 1975.
GLP:	Yes
Test substance:	As prescribed by 1.1-1.4, purity: >90%
Remarks:	Test fish were obtained from Spring Creek Trout Hatchery in Lewistown, Montana. Test fish were held in culture tanks on a 16-hour daylight photoperiod and observed for at least 14 days prior to testing. A daily record of fish observations was maintained during the holding period, during which time the fish were fed a standard diet of commercial fish food until 48 hours prior to testing, when feeding was stopped. A 48-hour range-finding test preceded the definitive study. Test fish used had a mean weight of 0.30 g and a mean standard length of 27 mm. The test was conducted in 5-gallon glass vessels containing 15 liters of laboratory well water. The 0-hour measured control water parameters of this dilution water were dissolved oxygen 9.6 mg/l and pH 8.0. The test vessels were kept in a water bath at 12°C. Test fish were acclimated to the dilution water and test temperature, and held without food for 48 hours prior to testing. Nanograde Acetone was used to prepare the test solutions and as the solvent control. Ten fish per concentration were placed in the testing vessels within 20 minutes of the addition of the test material aliquots. The compound was tested over a range from 100 to 1000 mg/ml. All concentrations were observed once every 24 hours for mortality and abnormal effects. Dissolved oxygen values and pH ranges were monitored during the testing and remained within acceptable limits of 74-91% saturation of dissolved oxygen and pH values ranged from 8.0 to 8.2. The ammonia concentrations were below the toxic limit. Hardness (CaCO3) was 255 ppm. As a quality check, test fish were challenged with Antimycin A. Statistical analysis of the

concentration vs. effect data was obtained by employing a computerized program developed by Stephan et al. This program calculated the LC50 statistic and its 95% confidence limits using the binomial, the moving average, and the probit tests.
The estimated 96Hr LC50 and 95% confidence limits were within the 95% confidence limits reported in the literature, indicating that the fish were in good condition.

Reference: Monsanto AB-83-017 Analytical Biochemistry Labs July 1983

Reliability: (1) Valid without restriction

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static
Closed system

Species: Daphnia magna

Exposure period: 48 hours

Results: EC_{50} (24h) = 13 mg/l
EC_{50} (48h) = 7.7 mg/l
NOEC = 1.8 mg/l

Analytical monitoring: No

Method: Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians.
EPA Ecological Research Series EPA-660/3-75-009 April 1975

GLP: Yes

Test substance: As prescribed by 1.1-1.4, purity: >90%

Remarks: The Daphnia magna used in the test were cultured at the ABC facilities. Adult Daphnia were fed the algae Selenastrum capricornutum at lest every three days prior to testing and supplemented with a suspension of trout chow. The bioassay was conducted in 250ml glass beakers containing 200 ml of ABC well water. Dissolved oxygen concentration was 9.3 ppm, pH was 8.2 and hardness (CaCO3) was 255 ppm. Vessels were kept at 20°C in a temperature-controlled area. Lighting was maintained at 50-70 foot-candles on a 16-hour daylight photoperiod. An initial range-finding experiment was carried out to determine the exposure concentrations for the definitive test. Dimethylformamide (DMF) was used as the solvent for the test solutions, and the experiment included both a control and a solvent control. The compound was tested over a range from 1.8 to 32 mg/l. Ten Daphnia, first instar less than 24 hours old, were selected for each test concentration. Daphnia in all concentrations were observed once every 24 hours for mortality and abnormal effects. Dissolved oxygen levels ranged from 8.0-6.3 mg/l (89-70% saturation) and pH (range 8.4-8.5) throughout the testing and were considered adequate and equivalent to those measurements in the control chamber. Statistical analysis of the concentration vs. effect data was obtained by employing a computerized program developed by Stephan et al. This program calculated the LC50 statistic and its 95% confidence limits using the binomial, the moving average, and the probit tests.

Reference: Monsanto AB-83-018 Analytical Biochemistry Labs July, 1983

Reliability: (1) Valid without restriction

***4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae**

Species:	Selenastrum capricornutum.
Endpoint:	Growth rate
Exposure period:	96 Hours
Results:	EC_{50} (96h) = >100 mg/l NOEC = 100 mg/l LOEC = Not determined
Analytical monitoring:	No
Method:	EPA Selenastrum capricornutum Algal Assay Test 1971 Closed system
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: >90%
Remarks:	In a study to determine the water quality effects of common lubrication additives, concentrations ranging from 1-100 mg/l of the test substance had no effect on algal growth.
Reference:	AMRL-TR-125:457-491 Scherfig, J and Dixon, P.S. Use of Unicellular Algae for Evaluation of Potential Aquatic Contaminants. Aerospace Medical Research Laboratory, 1975
Reliability:	(4) Not assignable - data from a secondary literature source

5. TOXICITY

***5.1 ACUTE TOXICITY**

5.1.1 ACUTE ORAL TOXICITY

Type:	LD_{50}
Species/strain:	Rats, Sprague-Dawley Albino
Value:	>7940 mg/kg bw
Sex:	Male/female
# of Animals:	10
Vehicle:	Corn Oil
Doses:	6310 or 7940 mg/kg bw
Method:	Single Oral Dose, Younger Laboratories Protocol, 1973
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: >90%
Remarks:	The test material was administered to 2 groups of male and female rats (5 animals/dose level) as a 20.0% suspension in corn oil. Dose levels were either 6310 or 7940 mg/kg body weight. Male rats had initial body weights of 230 grams: females had initial body weights of 210-220 grams. Only clinical signs noted were slightly reduced appetite and activity for one to two days. All animals survived until sacrifice on Day 14. All viscera appeared normal at necropsy.

Dose mg/kg	Mortalities-Male	Mortalities-Female	Combined
6310	0/2	0/3	0/5
7940	0/3	0/2	0/5

Reference: Monsanto YO-74-017 Younger Laboratories, March 11, 1974
Reliability: (2) Valid with restrictions – age of study, lack of method detail

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_{50}
Species/strain: Rabbits, New Zealand Albino
Value: >7940 mg/kg bw
Sex: Male/female
# of Animals: 3
Vehicle: Corn Oil
Doses: 5010 or 7940 mg/kg bw
Exposure Time: 24 Hours
Method: Single Dermal Dose, Younger Laboratories Protocol, 1973
GLP: No data
Test substance: As prescribed by 1.1-1.4, purity: >90%
Remarks: The test substance, as a 40.0% suspension in corn oil, was applied to the shaved skin of two groups of male and female rabbits for 24 hours as single dermal application at dose levels of 5010 or 7940 mg/kg/body weight. Mean body weight of males was 2.5 kg, and female 2.2 kg. The test material was held in place by means of an occlusive wrap of latex rubber and secured by bandaging and elastic tape. The occlusive wrap was removed after 24 hours and the excess material was wiped from the test animal. Clinical observations were made three times during the first eight hours after dosing, and twice daily thereafter until sacrifice. Clinical signs of toxicity included slightly reduced appetite and activity for one or two days. There were no mortalities at any dose level. All animals survived until sacrifice on Day 14. Gross autopsy reports indicated that all viscera appeared normal.

Dose mg/kg	Mortalities-Male	Mortalities-Female	Combined
5010	0/1	----	0/1
7940	0/1	0/1	0/2

Reference: Monsanto YO-74-017 Younger Laboratories, March 11, 1974
Reliability: (2) Valid with restrictions – age of study, lack of method detail

5.2.1 SKIN IRRITATION/CORROSION

Species/Strain: Rabbits, New Zealand Albino
Results: Not Irritating
Classification: Not Irritating
Method: Draize, J.H., Woodard, G., and Calvery, H.O., 1944
GLP: No data
Test substance: As prescribed by 1.1-1.4, purity: >90%
Remarks: 0.5 grams of the test substance, as a finely ground powder moistened with water, was applied to the shaved dorsal areas of six albino rabbits. The test material was applied to the skin under 1" square gauze patches and held in contact with the skin by means of an occlusive wrap of latex rubber secured by bandaging and elastic

tape. The occlusive wrap and gauze patches were removed after 24 hours. Dermal irritation was scored by the Draize Method, and results were recorded 24, 48, 72 and 168 hours after topical application. The Primary Irritation Index was calculated by averaging the mean scores at 24 and 72 hours. The Primary Irritation Index was found to be 0.0 on a scale of 0.0-8.0. All animals scored zero at each observation period.

Reference: Monsanto YO-74-017 Younger Laboratories, March 11, 1974
Reliability: (2) Valid with restrictions – age of study, lack of method detail

5.2.2 EYE IRRITATION/CORROSION

Species/strain: Rabbits, New Zealand Albino
Results: Slightly Irritating
Classification: Not Irritating
Method: Draize, J.H., Woodard, G., and Calvery, H.O., 1944
GLP: No data
Test substance: As prescribed in 1.1-1.4, purity: >90%
Remarks: 100 mg of the test substance, as a finely ground powder, was applied to one eye of six albino rabbits. The other eye was not treated and served as a control. The cornea, iris and conjuntivea were examined immediately after treatment, and then at intervals of 10 minutes, 1 hour, and then at 24, 48, 72 and 168 hours.
The Draize Method was used for scoring eye irritation. Immediate findings were slight discomfort. At 10 minutes, slight erythema and slight discharge were noted. At 24 hours, there was slight erythema and moderate discharge in all test animals. At 48 hours, two of six animals exhibited slight erythema and slight discharge. The average Draize score for 24, 48 and 72 hours was calculated for each animal and then averaged over the six animals. The average Draize score was 1.3 on a scale from 0-110. All signs of irritation had subsided by the third day after exposure.
Reference: Monsanto YO-74-017 Younger Laboratories, March 11, 1974
Reliability: (2) Valid with restrictions – age of study, lack of method detail

***5.4 REPEATED DOSE TOXICITY**

***5.5 GENETIC TOXICITY IN VITRO**

A. BACTERIAL TEST

Type: Ames Bacterial Reverse Gene Mutation
System of testing: Salmonella typhimurium, TA1535, TA1537, TA1538, TA98, TA100
Concentration: 0.1, 1.0, 10.0, 100.0 or 500.0 micrograms per plate
Metabolic activation: With and without
Results:
Cytotoxicity conc: With metabolic activation: 500 ug/plate
Without metabolic activation: 500 ug/plate
Precipitation conc: Not Determined
Genotoxic effects:
With metabolic activation: Negative
Without metabolic activation: Negative

Method:	Ames Mutagenicity Plate Test (Overlay Method) 1975
GLP:	No data
Test substance :	As prescribed by 1.1-1.4, purity: >90%
Remarks:	The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The *Salmonella typhimurium* strains used for this experiment were obtained from Dr. Bruce Ames. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. Chemicals used as positive controls for the non-activation assays were methylnitrosoguanidine (MNNG), 2-nitrofluorene (NF) and quinacrine mustard (QM). Positive control chemicals used for the activation assays were 2-anthramine (ANTH), 2-acetylaminofluorine (AAF) and 8-aminoquinoline (AMQ). Dimethylsulfoxide (DMSO) was used as the solvent and the solvent control. Analysis included Bartlett's test for homogeneity of variance, and comparison of treatments with controls using within-levels pooled variance and a one-sided t-test. Grubbs' test was performed to determine if outliers were present. The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.
Reference:	Monsanto BIO-76-281 Litton Bionetics, Inc. December 30, 1976
Reliability:	(1) Valid without restriction

B. NON-BACTERIAL IN VITRO TEST

Type:	Mitotic Recombination Assay
System of testing:	Saccharomyces cerevisiae, D4
Concentration:	0.1, 1.0, 10.0, 100.0 or 500.0 micrograms per plate
Metabolic activation:	With and without
Results:	
Cytotoxicity conc:	With metabolic activation: 500 ug/plate Without metabolic activation: 500 ug/plate
Precipitation conc:	Not Determined
Genotoxic effects:	
	With metabolic activation: Negative Without metabolic activation: Negative
Method:	Ames Mutagenicity Plate Test (Overlay Method) 1975
GLP:	No data
Test substance :	As prescribed by 1.1-1.4, purity: >90%
Remarks:	The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. The chemical used as the positive control for the non-activation assay was

methylnitrosoguanidine (MNNG) at 10 ug/plate. Positive control chemical used for the activation assay was DMNA at 100 micromoles/plate. Dimethylsulfoxide (DMSO) was used as the solvent and the solvent control. Analysis included Bartlett's test for homogeneity of variance, and comparison of treatments with controls using within-levels pooled variance and a one-sided t-test. Grubbs' test was performed to determine if outliers were present. The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.

Reference: Monsanto BIO-76-281 Litton Bionetics, Inc. December 30, 1976
Reliability: (1) Valid without restriction

Type: Sister Chromatid Exchange in Mammalian Cells
System of testing: Chinese Hamster Ovary (CHO) cells
Concentration: No data
Metabolic activation: With and Without
Results:
Cytotoxicity conc: With metabolic activation: No data
Without metabolic activation: No data
Precipitation conc: Not Determined
Genotoxic effects:
With metabolic activation: Negative
Without metabolic activation: Negative
Method: OECD 479 In vitro Sister Chromatid Exchange Assay In Mammalian Cells (1986)
GLP: Yes
Test substance: As prescribed by 1.1-1.4, purity: >90%
Remarks: Octylated Diphenylamine was one of 46 chemicals tested for the ability to induce sister chromatid exchanges (SCE) and chromosomal aberrations (AB) in cultured Chinese hamster ovary (CHO) cells using the standard OECD 479 protocol with and without exogenous metabolic activation. The test article did not induce a positive response for SCE and AB with and without metabolic activation.
Reference: Loveday, K.S., Anderson, B.E., Resnick, M.A., Zeiger, E. Chrosome Aberration and Sister Chromatic Exchange Tests in Chinese Hamster Ovary Cells in vitro. V: Results with 46 Chemicals., Environ. Mol. Mutagen. (1990), 16(4), 272-303
Reliability: (4) Not assignable - data from a secondary literature source

Type: Cytogenetic Assay, Mammalian Chromosome Aberration
System of testing: Chinese Hamster Ovary (CHO) and Chinese Hamster Lung (CHL) cells
Concentration: No data
Metabolic activation: With and Without
Results:
Cytotoxicity conc: With metabolic activation: No data
Without metabolic activation: No data
Precipitation conc: No data
Genotoxic effects:
With metabolic activation: Negative

Without metabolic activation: Negative

Method: In vitro Mammalian Chromosome Aberration Test (OECD 473)

GLP: Yes

Test substance: As prescribed by 1.1-1.4, purity: >90%

Remarks: Octylated diphenylamine was one of 25 chemicals tested for the induction of chromosomal aberrations in two cultured mammalian cell systems – CHO and CHL. In tests conducted with the S9 activation mix, octylated diphenylamine was negative in both. In tests conducted without the S9 mix, octylated diphenylamine was also negative in both cell systems.

Reference: Sofuni, T., Matsuoka, A., Sawada, M., Ishidate, J.,Zeiger, E., Shelby, M. Mutation Res.(1990), 241(2), 175-213

Reliability: (4) Not assignable - data from a secondary literature source

*** 5.6 GENETIC TOXICITY IN VIVO**

Type: Mammalian Germ Cell Mutation

Species/strain: Mice and rats

Sex: Male/Female

Route of Administration: Oral gavage

Exposure period: No data

Doses: No data

Results:

Effect on mitotic index or P/N ratio: No data

Genotoxic effects: Weak Positive

Method: Rat Dominant Lethal Assay and Unscheduled DNA Synthesis

GLP: No data

Test substance: As prescribed by 1.1-1.4, purity: >90%

Remarks: Weak positive evidence of activity of the test article was noted, but the effects were judged to be marginal. The authors concluded that no clear trends showing a significant potential for genetic effects could be established, and that the type of weak positive data obtained did not support the conclusion that the test article represents a serious genetic or carcinogenic risk to mammals.

Reference: Brusnick, D., Matheson, D. Litton Bionetics, Inc. AMRL-TR-78-46, Report (1978)

Reliability: (4) Not assignable - data from a secondary literature source

***5.8 TOXICITY TO REPRODUCTION**

***5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY**

Species/strain: Other: Chicken embryos, White Leghorn

Sex: Male/Female

Route of Administration: Injection into egg air chamber

Duration of the test: 11 days (Day 3 – Day 14)

Exposure period: 11 days

Frequency of treatment: Once on Day 3

Vehicle: Acetone, 5 ul

Doses: 0-1.0 umoles/egg

Control group: Yes

Concurrent vehicle

NOEL teratogenicity : 1.0 umoles/egg

Results:	Foetal data: No effect on embryos. No dose-response curve. No median effective dose could be calculated do to lack of effects
Method:	Other: Application of the chicken embryo in testing for embryotoxicity, Korhonen et al., 1982
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: commercial grade
Remarks:	Three day (72-76 hr) chicken embryos were selected by candling. The test compound, in 5 ul acetone, was injected into the heart of the embryo. Two days after injection, the eggs were candled again. Eggs containing dead embryos were counted and discarded. The remaining eggs were candled every second or third day. Those containing dead embryos were opened, and the embryos examined for external malformations and for the stage of development. Incubation was terminated after 11 days (total incubation time of 14 days), and the remaining eggs were opened and inspected for survival and external malformations. Embryos were classified according to time of death, stage of development and type of malformations. LD50 and ED50 values were calculated according to the method of Rosiello, et al. (1977). The test compound did not induce any effects (early death, defects or malformations) above those of the background (vehicle) acetone.
Reference:	Kohornen, et al., Institute of Occupational Health, Finland, 1983
Reliability:	(2) Valid with restrictions – avian rather than mammalian study

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type:	Teratogenicity Frog embryos and larvae
Results:	Several additives commonly found in aviation lubricants were tested for their potential effects as runoff pollutants in surface waters around Air Force bases. Dioctyldiphenylamine in water had no deleterious effects on the development of frog embryos or larvae under the test conditions.
Remarks:	None
Reference:	Greenhouse, G.A. (1975) Effects of Pollutants on Embryos and Larvae of Frogs: A System for Evaluating the Teratogenic Effects of Compounds in Freshwater Environments. Aerospace Medical Research Laboratory, Tech Report AMRL-TR-125:493-511
Reliability:	(4) Not assignable - data from a secondary literature source

B. Toxicodynamics, toxicokinetics

* 5.11 EXPERIENCE WITH HUMAN EXPOSURE

6. REFERENCES

1) ASTM D-1519 / Flexsys Standard Physical Methods of Analysis
2) Monsanto Company MSDS Flectol ODP May 1971
3) FF97.8-1 Flexsys Standard Physical Method of Analysis 1997

4) Monsanto Company. Toxicology Profile Flectol ODP. Original, November 15, 1988 by J.W. Barnett, Jr. Update November 10, 1992 by C.E. Healy
5) EPIWIN/KOWWIN v1.66
6) Hawley,G.G. The Condensed Chemical Dictionary, 1977.313
7) EPIWIN/WSKOW v1.40
8) EPIWIN/HENRYWIN v3.10
9) EPIWIN/AOPWIN v1.90
10) EPIWIN/PCKOCWIN v1.66
11) Handbook of Chemical Property Estimation Methods, 1990
12) EPISUITE/EPIWIN v3.10
13) EPIWIN/BCFWIN v2.14
14) Acute Toxicity of Flectol ODP to Bluegill Sunfish (Lepomis machrochirus) Monsanto AB-83-016 Analytical Biochemistry Laboratories July 27, 1983
15) Acute Toxicity of Flectol ODP to Rainbow Trout (Salmo gairdneri) Monsanto AB-83-017 Analytical Biochemistry Laboratories July 22, 1983
16) Acute Toxicity of Flectol ODP to Daphnia magna Monsanto AB-83-018 Analytical Biochemistry Laboratories July 28, 1983
17) AMRL-TR-125:457-491 Scherfig, J and Dixon, P.S. Use of Unicellular Algae for Evaluation of Potential Aquatic Contaminants. Aerospace Medical Research Laboratory, 1975
18) Acute Oral Toxicity of Flectol ODP to Albino Rats, Monsanto YO-74-017 Younger Laboratories, March 11, 1974
19) Acute Dermal Toxicity of Flectol ODP to Albino Rabbits, Monsanto YO-74-017 Younger Laboratories, March 11, 1974
20) Primary Skin Irritation of Flectol ODP to Albino Rabbits, Monsanto YO-74-017 Younger Laboratories, March 11, 1974
21) Primary Eye Irritation of Flectol ODP to Albino Rabbits, Monsanto YO-74-017 Younger Laboratories, March 11, 1974
22) Mutagenicity of Flectol ODP, Monsanto BIO-76-281 Litton Bionetics, Inc. December 30, 19761814)
23) Loveday, K.S., Anderson, B.E., Resnick, M.A., Zeiger, E. Chrosome Aberation and Sister Chromatic Exchange Tests in Chinese Hamster Ovary Cells in vitro. V: Results with 46 Chemicals., Environ. Mol. Mutagen. (1990), 16(4), 272-303
24) A Comparison of Chromosome Aberation Induction by 25 Compounds Tested by Two Chinese Hamster Cell (CHL and CHO) Systems in Culture. Sofuni, T., Matsuoka, A., Sawada, M., Ishidate, J.,Zeiger, E., Shelby, M. Mutation Res.(1990), 241(2), 175-213
25) Mutagen and Oncogen Study on 4,4-Dioctyldiphenylamine, Brusnick, D., Matheson, D. Litton Bionetics, Inc. AMRL-TR-78-46, Report (1978)
26) Greenhouse, G.A. (1975) Effects of Pollutants on Embryos and Larvae of Frogs: A System for Evaluating the Teratogenic Effects of Compounds in Freshwater Environments. Aerospace Medical Research Laboratory, Tech Report AMRL-TR-125:493-511
27) Kohornen, A, Hemminki, K., Vainio, H., Toxicity of rubber chemicals towards three-day chicken embryos, Institute of Occupational Health, Finland. Scand. J. Work Environ. Health 9, 115-119, 1983

I U C L I D

D a t a S e t

Existing Chemical	ID: 36878-20-3
CAS No.	36878-20-3
EINECS Name	bis(nonylphenyl)amine
EINECS No.	253-249-4
Molecular Formula	C30H47N

Producer Related Part

Company:	Epona Associates, LLC
Creation date:	11-APR-2001

Substance Related Part

Company:	Epona Associates, LLC
Creation date:	11-APR-2001

Printing date:	02-NOV-2001
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Reliability (profile):	Reliability: 1, 2
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 Melting Point
-

2.2 Boiling Point
-

2.4 Vapour Pressure
-

2.5 Partition Coefficient
-

2.6.1 Water Solubility
-

3.1.1 Photodegradation
-

3.1.2 Stability in Water
-

3.3.1 Transport between Environmental Compartments
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to Test substance
Contact time: 28 day
Degradation: = 8 % after 28 day
Result: under test conditions no biodegradation observed
Controlsubstance: Benzoic acid, sodium salt

Deg. Product: no
Method: OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year: 1997 GLP: yes
Test substance: other TS
Remark: Control substance: >60% in 3 days
Innoculum: Return activated sludge from domestic wastewater treatment plant.
Result: The test substance showed a low biodegradation rate (8.0%) in 28 days. The reference substance, sodium benzoate, reached a level of 82.3% in the same test period.
Test conditions:Inoculum: The supernatant from the homogenized activated sludge was used as inoculum. The inoculum was pre-adapted to the test material for 14 days during which the test substance was added incrementally at concentrations equivalent to 4, 4 and 8 mg carbon/L on days 0, 7, and 12, respectively. The targeted microbial level in the test mixture was 10,000 to 1,000,000 cells/mL. Concentration of test chemical: Test substance concentration was approximately 100 mg/L mineral medium, giving at least 50 to 100 mg ThOD per L medium.
No organic solvents were used to facilitate the dispersion of the test material. The test substance was weighed onto a teflon coupon and introduced into the medium. Temp of incubation: 23 $\pm$ 1°C. Dosing procedure: A measured volume of the inoculated mineral medium containing approximately 100 mg/L test substance is continuously stirred in a closed system for 28 days.
Sampling frequency: The oxygen uptake were monitored continuously and recorded every 4 hours throughout the test. Controls: Yes (blank and positive controls per guideline); abiotic and toxicity checks were not included. Sodium benzoate was used as the positive control. Analytical method: Oxygen uptake was measured using a BI-1000 electrolytic respirometer system. Method of calculating measured concentrations: N/A.
Other: The inoculum was pre-adapted to the

test substance for 14 days.
Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-
Reliability: (1) valid without restriction
02-NOV-2001 (1)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: semistatic
Species: *Pimephales promelas* (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: c > 10000
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1993 GLP: yes
Test substance: other TS
Remark: Statistical methods were not used as there were no deaths at the highest test concentration.
Test conditions: Test Organisms: Source - Aquatic Research Organisms, Hampton, New Hampshire; Age- Juvenile; Length - not determined; Wet weight - 0.41 g; Loading rate - 0.27 g/L; Pretreatment - none, fish were acclimated to the test conditions for 14 days prior to start of test. Test System: The static acute screening test was conducted using nominal test concentrations of 1,000 mg/L, 5,000 mg/L and 10,000 mg/L. The test substance was directly added to the dilution water and no solvent was used. The test was conducted in 20 L, polyethylene-lined, glass aquaria that contained 15 L of test solution. 10 fish were used for each test concentration (no replicates were used). Test media was renewed after 48 hours. The fish were not fed during the test. Dilution Water: Source - Dechlorinated tap water; Hardness - Water adjusted to a hardness of 172 - 176 mg/L as $CaCO_3$; Analysis - Water was free of measurable quantities of pesticides; Water chemistry in test: DO (% Saturation) - 92 to 104%; pH - 7.2 to 8.0Test Temperature (°C) - 22 $\pm$ 1Test Levels: Control, 1,000, 5,000 and 10,000 mg/L
Test method: U.S. EPA TSCA 797.1400 (1985)
Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-
Remark: A sheen of insoluble material was observed in all non-control test vessels.
Reliability: (1) valid without restriction
02-NOV-2001 (4)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: semistatic
Species: *Mysidopsis bahia* (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: c = 250
EC50: c = 733
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute

Immobilisation Test"
Year: 1991 GLP: yes
Test substance:
Method: Test method: Static renewal with WAF
Remark: EL50's were calculated using standard statistical methods from Stephan (1983). Results: Effect concentrations based on nominal loading rates. Control response was satisfactory (>90% survival and no sublethal effects).
Results: Mysids exposed to 600 mg/L were lethargic and exhibited erratic swimming from 48 to 96 hours. No other sublethal effects were observed in any test vessel during the 96 hour exposure.
Test conditions: Test species: Juvenile mysids less than 24-hours old were produced from laboratory in-house culture. Test System: The test was conducted using the water accommodated fraction (WAF) of nominal test concentrations. Individual WAFs were prepared by adding a measured weight of test material to a measured volume of dilution water (1-L) in a glass vessel and stirring for 24 hours. Following the mixing period, the test solutions were allowed to stand for 1 hour before the water phase was siphoned off. The siphoned water phase (i.e., WAF) was used for the aquatic toxicity test.Test conditions: A 2-L glass beaker that contained 1 L of test solution was used per treatment. The test vessels were loosely covered to reduce entry of dust, etc. Mysids were fed newly hatched *Artemia salina nauplii* once or twice daily during the test. Dilution water: Seawater collected from the Atlantic Ocean in Hampton, New Hampshire was used. Water was adjusted to a salinity of 20 parts per thousand and aerated. Water was free of pesticides and PCBs at the detection limit. Water chemistry; pH - 8.1; TOC - 3.9 to 8.2. Element: Immobilization/mortality. Test Temperature (°C) - 24 $\pm$ 1. Test Levels: Control, 150, 250, 400, 600 and 1,000 mg/L nominal test concentrations. The WAF was used for testing. 10 mysids per test vessel (2 replicates per test concentration were used).
Test method: US EPA TSCA #797.1300 (1985)
Reliability: (1) valid without restriction
02-NOV-2001 (2)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: *Selenastrum capricornutum* (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
NOEC: c = 33
EL50 : c = 600
EL0 : c = 870

Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1997 GLP: yes
Test substance: other TS
Remark: Effects were determined to be algistatic based on the rapid re-growth of an aliquot of cells taken from 500 mg/L cultured in fresh control media.
EL50s were calculated using Standard statistical methods from Stephan (1983)
Method: US EPA TSCA, 797.1050
Test conditions: Test Species: Cells taken from a log-growth phase in-house culture of *Selenastrum capricornutum* that was originally purchased from University of Texas at Austin alga collection. Test System: Individual WAFs were prepared for each test level and renewed daily. Individual WAFs were prepared by adding a measured weight of test material to a measured volume of dilution water (1-L) in a glass vessel and stirring for 24 hours. Following the mixing period, the test solutions were allowed to stand for approximately 4 hours before the water phase was siphoned off. The siphoned water phase (i.e., WAF)was used for the aquatic toxicity test. Test Conditions: A static test was conducted; i.e., there was no daily renewal of test solution. Three 100-mL replicates per treatment, inoculum ~10,000 cells/mL. The 250-mL Erlenmeyer flasks were stoppered with foam plugs to reduce entry of dust, etc. During the test all treatment and control flasks were randomly placed on an orbital shaker adjusted to approximately 100 cycles per minute under constant light (24 hours/day). Daily cell counts were made visually by means of direct microscopic examination with a hemocytometer. Light: Cool-white fluorescent lights provided a light intensity of 370 to 380 foot-candles 24-h per day. Test temperature (°C) - 24 $\pm$ 1. Dilution Water: Sterile enriched alga growth media adjusted to pH 7.5. Particulate matter ranged from <10 mg/L at the start of the test to 29 mg/L at the end of the test. pH ranged from 7.6 - 8.1 at 0-hour and 9.0 - 9.7 after 96 hours. Test Levels:
Control, 0.3, 3.3, 33, 330 and 3,300 mg/L WAF loading rates.
Test substance: Benzamine, ar-nonyl-N-(nonylphenyl)-
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
02-NOV-2001 (3)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity
-

5.1.2 Acute Inhalation Toxicity
-

5.1.3 Acute Dermal Toxicity
-

5.1.4 Acute Toxicity, other Routes
-

5.4 Repeated Dose Toxicity
-

5.5 Genetic Toxicity 'in Vitro'
-

5.6 Genetic Toxicity 'in Vivo'
-

5.8 Toxicity to Reproduction
-

5.9 Developmental Toxicity/Teratogenicity
-

6. References

(1) Biodegradability study of benzenamine, ar-nonyl-N-(nonylphenyl)- using batch processing respirometry test. Ricerca Inc., 19 Aug 1998.

(2) Acute toxicity of the water accommodated fraction (WAF) of benzenamine, ar-nonyl-N-(nonylphenyl)- to the mysid Mysidopsis bahia. EnviroSystems,, 04 October 1991.

(3) Acute toxicity of the water accommodated fraction (WAF) of benzenamine, ar-nonyl-N-(nonylphenyl)- to the freshwater algae Selenastrum capricornutum. Wilbury Labs, 11 Sept 1997.

(4) Acute toxicity of benzenamine, ar-nonyl-N-(nonylphenyl)- to the fathead minnow, Pimephales promelas. Wilbury Labs, 15 Jan 1993.

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, 2-ethyl-N-(2-ethyl[phenyl)-, (tripropenyl) derivatives. . . . . .

CAS No. 68608-77-5

Sponsor Country : . . . . . .

DATE: . . . . . .

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 68608-77-5

B. Name *(IUPAC name)*

***C. Name** *(OECD name)*

†D. CAS Descriptor Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivatives

E. EINECS-Number 271-800-7

F. Molecular Formula

***G. Structural Formula**

H. Substance Group

I. Substance Remark

J. Molecular Weight 225-479

1.02 OECD INFORMATION

A. Sponsor Country: United States

B. Lead Organisation:

Name of Lead Organisation: Noveon, Inc.
Contact person: Robert K. Hinderer, Ph.D
Address:
Street: 9911 Brecksville Rd.
Postal code: 44141-3247
Town: Cleveland
Country: U.S.A.
Tel: (216)447-5181
Fax: (216)447-5760

C. **Name of responder** *(Information on a responder should be provided when companies respond to Lead Organisation or SIDS Contact Points.)*

Name:
Address:
Street:
Postal code:
Town:
Country:
Tel:
Fax:

1.1 GENERAL SUBSTANCE INFORMATION

A. **Type of Substance**

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ]; petroleum product [ ]

B. **Physical State** *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. **Purity** *100 %*

1.2 SYNONYMS Good-rite® NEPA; Vanlube® NA; Goodrite® 3185

1.3 IMPURITIES

CAS No:
EINECS No:
Name:
Value:
Remarks:

1.4 ADDITIVES

CAS No:
EINECS No:
Name:
Value:
Remarks:

2. <u>PHYSICAL-CHEMICAL DATA</u>

***2.1 MELTING POINT**

Value: °C
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: *[e.g. OECD, other* .
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

***2.2 BOILING POINT**

Value: 443.18 – 547.61 °C
Pressure: at hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products…
Reference: EPIWIN

†2.3 DENSITY (relative density)

Type: Bulk density **[ ]**; Density **[ ]**; Relative Density **[x] Specific Gravity**
Value: 0.915-0.955
Temperature: °C
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Specific Gravity
Reference: Noveon, Inc. MSDS 2001

***2.4 VAPOUR PRESSURE**

Value: 2.35E-008 to 9.18E-012 hPa
Temperature: 25 °C
Method: calculated **[x]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products…
Reference: EPIWIN

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$**

Log Pow: 9.84
Temperature: °C
Method: calculated **[x]**; measured **[ ]** EPIWIN.
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products...
Reference: EPIWIN

***2.6 WATER SOLUBILITY**

A. Solubility

Value: 2.35e-005 to 5.85e-010
Temperature: 25 °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Based on the two reaction products that are 90+% of all reaction products...
Reference: EPIWIN

Solubility

Value: **Insoluble**
Temperature: °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference: Noveon, Inc. MSDS 2001

B. pH Value, pKa Value

pH Value:
Concentration:
Temperature: °C
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
pKa value at 25°C
Remarks:
Reference:

2.7 FLASH POINT *(liquids)*

Value: 213 °C

Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.8 AUTO FLAMMABILITY *(solid/gases)*

Value: °C
Pressure: hPa
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**; More sensitive to friction than m-dinitrobenzene **[ ]**; More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

†2.12 OXIDATION: REDUCTION POTENTIAL

Value: mV
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

B. Other data

Results:
Remarks:
Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: nm
Relative intensity:
Spectrum of substance: nm
Concentration of Substance:
Temperature: °C
Direct photolysis:
Half life: 0.05 days to 0.048 days
Degradation: % (weight/weight) after . . . . . (exposure time)
Quantum yield:
Indirect Photolysis:
Type of sensitizer:
Concentration of sensitizer:
Rate constant (radical): cm^3/molecule*sec
Degradation:
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks: Based on the two reaction products that are 90+% of all reaction products...
Reference: EPIWIN

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: at pH at °C
Degradation: at pH at °C after (exposure time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration:
Soil temperature: °C
Soil humidity:
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year
Content of clay etc.: Clay %, Silt %, Sand %
Organic Carbon:
Soil pH:
Cation exchange capacity:
Microbial biomass:
Dissipation time: DT 50 :
DT 90 :
Dissipation : % after (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

*3.2 MONITORING DATA (ENVIRONMENTAL)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media:
Results:
Remarks:
Reference:

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media:
Method:
Results:
Remarks:
Reference:

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPIWIN
Results: Air 0.0424-0.0393%, 1.2-1.15 half-life, 1000 kg/hr emissions
Water 4.34-4.31%, 1.48e+003 half-life, 1000 kg/hr emissions
Soil 56.1-56.4%, 1.48e+003 half-life, 1000 kg/hr emission
Sediment 39.5-39.2%, 1.48e+003 half-life, 1000 kg/hr emission
Remarks: Based on the two reaction products that are 90+% of all reaction products...
Reference: .EPIWIN

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results:
Remarks:
Reference:

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
. . . . . % after . . . . . (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) . . . . . % in . . . . . (time)
Method: *[e.g. OECD, other (with the year of publication or updating of the method*
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5
Method:
Concentration: related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: mg O_2/l
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method:
Value: mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD_5/COD:
Remarks:
Reference:

3.7 BIOACCUMULATION

Species:
Exposure period:
Temperature: °C
Concentration:
BCF:
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.8 ADDITIONAL REMARKS

A. Sewage treatment

Results:
Remarks:
Reference:

B. Other information

Results:
Remarks:
Reference:

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: LC_{50} (24h) = ... mg/l
LC_{50} (48h) = ... mg/l
LC_{50} (72h) = ... mg/l
LC_{50} (96h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**;
open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

B. Other aquatic organisms

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:	
Exposure period:	
Results:	EC_{50} (24h) = ... mg/l EC_{50} (48h) = ... mg/l EC_{xx} (..h) = ... mg/l NOEC = ... mg/l
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[ ]**
Method:	
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: .	purity:
Remarks:	
Reference:	

***4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae**

Species:	
Endpoint:	Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period:	
Results:	EC_{50} (. . . . . h) = ... mg/l EC_{xx} (. . . . . h) = ... mg/l NOEC = ... mg/l LOEC = ... mg/l
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[ ]**
Method:	
	open-system **[ ]**; closed-system **[ ]**
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:	purity:
Remarks:	
Reference:	

4.4 TOXICITY TO BACTERIA

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:
Exposure Period:
Results: EC_{50} (. . . h) = ... mg/l
EC_{xx} (. . . h) = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (..d) = ... mg/l
EC_{xx} (..d) = ... mg/l
NOEC = ...mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (. . . . . h) = ... mg/l
EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species:
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (. . . . . d) = ... mg/kg
EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

(b)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

(c)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

Results: Substance:
Species or ecosystem studied:
Effects monitored:
Results:
Chemical analysis:
Remarks:
Reference:

4.8 BIOTRANSFORMATION AND KINETICS

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results:
Remarks:
Reference:

4.9 ADDITIONAL REMARKS

Results:
Remarks:
Reference:

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 [ ]; LD_{100} [ ]; LD_{50} [**x**]; LDL_0 [ ]; Other [ ]
Species/strain: Rat/Charles River strain (COBS)
Value: >34,600 mg/kg b.w.:
Discriminating dose:
Method:
GLP: Yes [ ] No [x] ? [ ]
Test substance:), Goodrite® 3185 , purity: 100%
Remarks: Based on range finding data groups of rats (2/sex/group) were administered 10,250, 15,380, 23,070, or 34,600 mg/kg via oral gavage. Animals were observed for toxic signs; body weights were recorded at the beginning of the study and at the end of the 14-day observation period. No mortality was observed at any of the doses.
Reliability: (2) Relable with restrictions.
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 [ ]; LC_{100} [ ]; LC_{50} [ ]; LCL_0 [ ]; Other [**x**]
Species/strain: Rats/Sprague-Dawley
Exposure time: 4 hrs
Value:
Method:
GLP: Yes [ ] No [**x**] ? [ ]
Test substance: .), Goodrite® 3185 , purity: 100%..
Remarks: A groups of rats (5/sex/group) was exposed to the test material via inhalation exposure. Animals were observed for toxic signs; body weights were recorded at the beginning of the study and at the end of the 14-day observation period. Because of the materials low volatility, no weight loss of the test material was noted. No deaths were observed.
Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 [ ]; LD_{100} [ ]; LD_{50} [ ]; LDL_0 [ ]; Other [ ]
Species/strain: Rabbit/New Zealand
Value: >3,000 mg/kg b.w.
Method:
GLP: Yes [ ] No [x] ? [ ]
Test substance: . Goodrite® 3185 purity: 100%
Remarks: The test material was applied to a shaved area on the backs of four rabbits and then covered with an impervious plastic sheeting. After 4 hours the test material was removed, and the sites were examined for local reactions. Animals were observed for toxic signs; body weights were recorded at the beginning of the study and at the end of the 14-day observation period. No

mortality was observed at any of the doses. Skin reactions were limited to mild erythema, desquamation, and edema. Only barely perceptible to slight erythema and desquamation were present at day 14.

Reliability: (2) Relable with restrictions.

Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Route of Administration: ..... i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time:
Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain:
Results: ..... Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: *(If possible, according to EC Directive 67/548/EEC)*
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.2.2 EYE IRRITATION/CORROSION

Species/strain: Rabbit/New Zealand
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[x]**;
Not irritating **[ ]**
Classification: *(if possible, according to EC Directive 67/548/EEC)*
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Test substance: . Goodrite® 3185 , purity: 100%

Remarks: The eye irritation study was patterned after the Draize method (1944). Only conjunctival reactions were observed and only at the 1 hour observation.

Reference: Industrial Bio-test Laboratories, Inc. (1973), BFGoodrich Sponsor (now Noveon, Inc.)

5.3 SKIN SENSITISATION

Type:
Species/strain:
Results: Sensitizing **[ ]**; Not sensitizing **[ ]**; Ambiguous **[ ]**
Classification:
Sensitizing **[ ]**; Not sensitizing **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*5.4 REPEATED DOSE TOXICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Post exposure observation period:
Dose:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL:
LOEL:
Results:
Method: **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Reference:

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: *Bacterial reverse mutation assay*

System of testing: *Salmonella typhimurium,* strains TA-1535, TA-1537, TA-98, TA-100 and . *Escherichia coli*, strain WP2uvrA-.
Concentration: 0, 50, 150, 1500, 5000 ug/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[x]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: None toxic
Without metabolic activation: None toxic
Precipitation conc: 1500 and 5000 ug/plate
Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[-]**
Without metabolic activation:	**[ ]**	**[ ]**	**[-]**

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*
OECD B14 in EC Directive 92/69/EEC
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: Vanlube NA, purity: ..100 %
Remarks: The *S. typhymurium* strains were obtained from the University of California (Berkeley), and the *E. coli* strain was obtained from the British Industrial Biological Research Association. Overnight subcultures of the stock cultures were prepared in nutrient broth and incubated at 37°C for approximately 10 hours. The test material was dissolved in acetone to prepare the test concentrations noted above. Vehicle and positive controls were run in parallel with the test material. The positive controls were as follows:

Non-activation
TA100: N-ethy-N'-nitrosoquanidine (ENNG), 3 µg/plate
TA1535: ENNG, 5 µg/plate
TA1537: 9-aminoacridine, 5 µg/plate
TA98: 4-nitroquinoline-1-oxide, 0.2 µg/plate
WP2uvrA$^-$: ENNG, 2 µg/plate
Activation (10% liver S9)
TA100: 2-Aminoantracene (2AA), 1 µg/plate
TA1535: 2AA, 2 µg/plate
TA1537: 2AA, 2 µg/plate
TA98: 2AA, 0.5 µg/plate
WP2uvrA$^-$: 2AA, 10 µg/plate

A preliminary toxicity study was conducted to select the appropriate dose levels. Five doses of the test material and the vehicle control (acetone) were tested in duplicate. In addition, 0.1 ml of the maximum concentration of the test material and 2 ml of the molten medium were overlayed onto an agar plate. After 48 hours incubation at 37°C the plates were assessed for revertant colonies.

Two experiments were conducted to assess reproducibility. A substance was considered positive if it induce a dose-related and statistically significant increase in mutation rate (at least twice the spontaneous reversion rate) in one or more strains with or without activation. (Note: In the event of two equivocal experiments a third experiment may be used.) To be considered negative the number of induced revetants compared to the spontaneous revertants should be less than two fold at each dose level employed, the intervals of which should be between two and five fold and extend to the

limits imposed by toxicity, solubility or up to the maximum recommended dose of 5000 ug/plate. (Note: In this case the limiting factor was the maximum recommended dose.)

No toxicity was observed to any of the strains. Precipitates were observed at 1500 ug/plate and 5000 ug/plate but did not interfere with scoring. No significant increase in the frequency of revetant colonies was recorded in any strain with or without activation, and the responses of the positive controls were satifactory.

Reliability: (1) Reliable without limitations

Reference: Safepharm Laboratories Project No. 860/026, 21 May 1997, Sponsor R.T. Vanderbilt Co., Inc.

Flag: Critical study for SIDS endpoint and acceptable for assessment

Type: Bacterial reverse mutation assay
System of testing: Salmonella typhimurium strains TA-1535, TA-1537, TA-1538, TA-98, TA-100
Concentration: 0.5 to 5,000 ug/plate
Cytotoxic Conc.: With metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)
Without metabolic activation: 0.5 to 100 ug/plate (little to no toxicity)
Metabolic activation: with and without
Result: negative
Method: other: according to other: according to Ames et al (1975) Mutation Res. 31:347-364; McCann et al. (1975) Proc. Nat. Acad. Sci. 72:5135-5139
Year: 1979 GLP: no data
Test substance: Good-rite® NEPA, purity: ..100 %
Remark: The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations.

Salmonella typhymurium strains TA-1535, TA-1537, TA-1538, TA-98 and TA-100 were obtained from Dr. Bruce Ames. All indicator strains were kept at 4ºC on minimal medium plates supplemented with a trace of biotin and an excess of histadine (Ames, 1980). In addition, the plates with the plasmid-carrying *Salmonella* strains (TA-98 and TA-100) were supplemented with 26µg/ml of ampicillin to ensure stable maintenance of the plasmid pKM101. "

The bacterial strains were cultured at 37ºC in Oxid Media #2 (nutrient broth), and Vogel Bonner Medium E with 2% glucose was used as the selective medium (Vogel and Bonner, 1956). The overlay agar was prepared according to the method of Ames et al (1975). S-9 liver homogenates, which were prepared from Aroclor 1254-induced and noninduced adult Sprague-Dawley male rats as described by Ames et al (1975, were prepared from Binetics Laboratory Products, Litton Bionetics, Inc. An S-9 mix was prepared by adding the following ingredients per milliliter of mix: 4 µmoles NADP (sodium salt), 5 µmoles D-glucose-6-phosphate, 8 µmoles $MgCL_2$, 33 µmoles KCL, 100 µmoles sodium phosphate buffer (pH 7.4), and 100 µl of rat liver S-9 fraction.

All tests were based on the methods of Ames et al (1975). Test compounds were dissolved in dimethylsulfoxide (DMSO). Solvent and positive controls are

summarized as follows: Positive controls for the non-activation assays were 1 ug/plate sodium azide for TA-1535 and TA-100, 50 ug/plate 9-aminoacridine for TA-1537, 10 µg 2-nitrofluorene for TA-1538 and TA-98. The positive control used for the activation assays was 2.5 ug/plate 2-anthramine.) "The highest dose was established as one which produced some toxicity.

Criteria which were used to determine whether a chemical was mutagenic were: 1) an increase in revertants in strains TA-1535, TA-1537, TA-1538 of three times the solvent control; 2) an increase in revertants in strains TA-98 and TA-100 of twice the solvent control; 3) reproducibility; and 4) a dose-related response, and a consistent pattern of response between strains derived from the same parental strain

Signed QA assurance statement provided

Reliability: (2) Relable with restrictions. Meets generally accepted scientific standards, well documented.

Reference: Litton Bionetics, Inc. Project No. 20988, September 1979, Sponsor BFGoodrich (now Noveon, Inc.).

B. NON-BACTERIAL IN VITRO TEST

Type:
System of testing:
Concentration:
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[ ]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation:
Without metabolic activation:.
Precipitation conc:
Genotoxic effects: .....
+ ? -
With metabolic activation: **[ ] [ ] [ ]**
Without metabolic activation: **[ ] [ ] [ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

* 5.6 GENETIC TOXICITY IN VIVO

Type:
Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Doses:
Results:
Effect on mitotic
index or P/N ratio:
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.7 CARCINOGENICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Postexposure observation period:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[ ]**
Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Post exposure observation period:
Premating exposure period: male: . . . . . , female: .....
Duration of the test:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Parental:
NOEL F1 Offspring:
NOEL F2 Offspring:
Results:
General parental toxicity:
Toxicity to offspring: *(weights of litter, postnatal growth, viability, etc.)*

Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Duration of the test:
Exposure period:
Frequency of treatment:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity:
NOEL teratogenicity :
Results:
Maternal general toxicity:
Pregnancy/litter data:
Foetal data:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type:
Results:
Remarks:
Reference:

B. Toxicodynamics, toxicokinetics

Type:
Results:
Remarks:
References:

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE . . . . . CHEMICAL

Benzenamine, N-phenyl-, reaction products with styrene and 2, 4, 4-trimethylpentene

CAS No. 68921-45-9

Sponsor Country :

DATE:

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. Cast number** 68921-45-9

B. Name *(IUPAC name)*
***C. Name** *(OECD name)*
†D. CAS Descriptor Benzenamine, N-phenyl-, reaction products with styrene and 2, 4, 4-trimethylpentene

E. EINECS-Number 272-940-1

F. Molecular Formula

***G. Structural Formula**

H. Substance Group

I. Substance Remark

J. Molecular Weight 225-633

1.02 OECD INFORMATION

A. Sponsor Country: United States

B. Lead Organisation:

Name of Lead Organisation: Noveon, Inc.
Contact person: Robert K. Hinderer, Ph.D.
Address:
Street: 9911 Brecksville Rd.
Postal code: 44141-3247
Town: Cleveland, Ohio
Country: U.S.A.
Tel: (216)447-5181
Fax: (216)447-5760

C. Name of responder

Name:
Address:
Street:
Postal code:
Town:
Country:
Tel:
Fax:

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [x]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [x]; solid **[ ]**

C. Purity *98%*

1.2 SYNONYMS Good-rite® 3190NT; Vanlube® SL; Vanlube® SL-HP

1.3 IMPURITIES

CAS No: 122-39-4
EINECS No:
Name: Diphenylamine
Value: <2%
Remarks:

CAS No: 100-42-5
EINECS No:
Name: Styrene
Value: <0.0003%
Remarks:

1.4 ADDITIVES

CAS No:
EINECS No:
Name:
Value:
Remarks:

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: °C
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

*2.2 BOILING POINT

Value: >198 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks:
Reference: Noveon, Inc. MSDS

BOILING POINT

Value: 392.71 TO 663.07 °C
Pressure: at . . . . . hPa
Decomposition: Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method: EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[x]**
Remarks: Range for the components
Reference: EPIWIN

†2.3 DENSITY (relative density)

Type: Bulk density **[ ]**; Density **[ ]**; Relative Density **[x] Specific Gravity**
Value: 0.97-1.01
Temperature: °C
Method
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference: Noveon, Inc. MSDS

***2.4 VAPOUR PRESSURE**

Value: 9.99E-007 to 1.9E-015 hPa
Temperature: °C
Method: calculated **[ ]**; measured **[ ]** EPIWIN

.
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Range for components
Reference: EPIWIN

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$**

Log Pow: 5.2
Temperature: Room Temperature, 21 °C
Method: calculated **[ ]**; measured **[** x **]**
OECD Section 1 N0. 107; EEC Annex V Test Guideline A.*., September 19, 1984
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Remarks: Concentrations of Vanlube SL-HP, extracted into water were measured by UV. Because the test material has a low solubility in water, accurate test concentrations are difficult to prepare. Thus the molar absorbtivity in water was assumed to be similar to that in n-octanol. The concentration of the test material in the octanol layer was approximately 0.8 molar. This concentration, higher than suggested in the guidelines, was necessary so

that enough test material would be extracted into water (about $5x10^{-6}$ molar) to be detectable by UV. The change in concentration of the test material in the n-octanol before and after extraction is so small that the initial concentration of the test material is taken to be the concentration at equilibrium.

The molecular weight of monooctyl diphenylamine, 281, was taken as a representative MW of the test material. .....

The Log Pow was determined to be 5.2.

Reliability: (2) Valid with limitations
Flag: Critical study for SIDS endpoint
Reference: BFGoodrich Co., Brecksville R&D Center, November 28, 1990 (now Noveon, Inc.)

PARTITION COEFFICIENT $log_{10}P_{ow}$

Log Pow: 5.45 to 15.13
Temperature: Room Temperature, 21 °C
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference: EPIWIN

***2.6 WATER SOLUBILITY** *(if more than one, identify the recommended value)*

Solubility

Value: Negligible
Temperature: °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference: Noveon, Inc. MSDS

Solubility

Value: 0.3889 to 1.869e-011
Temperature: 25 °C
Description: Miscible **[ ]**; Of very high solubility **[ ]**;
Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**;
Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method: EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks: Range for components
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: EPIWIN

2.7 FLASH POINT *(liquids)*

Value: 180 °C
Type of test: Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference: Noveon, Inc. MSDS

2.8 AUTO FLAMMABILITY *(solid/gases)*

Value: °C
Pressure: hPa
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.9 FLAMMABILITY

Results: Extremely flammable **[ ]**; Extremely flammable - liquified gas **[ ]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.10 EXPLOSIVE PROPERTIES

Results: Explosive under influence of a flame**[ ]**;
More sensitive to friction than m-dinitrobenzene **[ ]**;
More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**;
Other **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

2.11 OXIDISING PROPERTIES

Results: Maximum burning rate equal or higher than reference mixture **[ ]**;
Vigorous reaction in preliminary test **[ ]**;
No oxidising properties **[ ]**; Other **[ ]**

Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

†2.12 OXIDATION: REDUCTION POTENTIAL

Value: mV
Method:

GLP: Yes **[ ]** No **[ ]** ? **[ ]** Remarks:
Reference:

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:
Reference:

B. Other data

Results:
Remarks:
Reference:

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type: Air **[x]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum: nm
Relative intensity:
Spectrum of substance: nm
Concentration of Substance:
Temperature: °C
Direct photolysis:
Half life: 0.053 days
Degradation: % (weight/weight) after (exposure time)
Quantum yield:
Indirect Photolysis:
Type of sensitizer:
Concentration of sensitizer:
Rate constant (radical): cm^3/molecule*sec
Degradation:
Method: calculated **[ ]**; measured **[ ]** EPIWIN
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference: EPIWIN

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life: at pH at °C

Degradation: at pH at °C after
(exposure time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.1.3 STABILITY IN SOIL

Type : Field trial **[ ]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel: Yes **[ ]** No **[ ]** ? **[ ]**
Concentration:
Soil temperature: °C
Soil humidity:
Soil classification: DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[ ]**
year
Content of clay etc.: Clay %, Silt %, Sand %
Organic Carbon:
Soil pH:
Cation exchange capacity:
Microbial biomass:
Dissipation time: DT 50 :
DT 90 :
Dissipation : % after (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

*3.2 MONITORING DATA (ENVIRONMENTAL)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[ ]**
Media:
Results:
Remarks:
Reference:

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.1 TRANSPORT

Type: Adsorption **[ ]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media:
Method:
Results:
Remarks:
Reference:

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**;
Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[ ]**
Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[x]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**
EPIWIN
Results: Air 0.0568% to 0.00992%, 1.27 hr to 1.23 hr. half-life, 1000 kg/hr
Water 13.5% to 1.26%, 900hr to 1.44e+003hr half-life, 1000 kg/hr
Soil 44% to 28.6%, 900hr to 1.44e+003, 1000 kg/hr
Sediment 42.5% to 69%, 3.6e+003 to 1.44e-004 half'life, 0 kg/hr .....
Remarks:
Reliability: (2) Valid with restrictions
Reference: EPIWIN

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

Results:
Remarks:
Reference:

*3.5 BIODEGRADATION

Type: aerobic **[ ]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[ ]**
Concentration of the chemical: . . . . . related to COD **[ ]**; DOC **[ ]**; test substance **[ ]**
Medium: water **[ ]**; water-sediment **[ ]**; soil **[ ]**; sewage treatment **[ ]**
Degradation: *(percentage reduction/exposure time)*
% after (time)
Results: *(see OECD Guidelines)* readily biodeg. **[ ]**; inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**
Kinetic (e.g. Zahn-Wellens-Test) % in (time)
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5
Method:
Concentration: related to COD **[ ]**; DOC **[ ]**; Test substance **[ ]**
Value: mg O_2/l

GLP: Yes **[ ]** No **[ ]** ? **[ ]**

COD
Method:
Value: mg O_2/g
GLP: Yes **[ ]** No **[ ]** ? **[ ]**

Ratio BOD_5/COD:
Remarks:
Reference:

3.7 BIOACCUMULATION

Species:
Exposure period:
Temperature: °C
Concentration
BCF:
Elimination: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
Type of test: calculated **[ ]**; measured **[ ]**
static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Reference:

3.8 ADDITIONAL REMARKS

A. Sewage treatment

Results:
Remarks:
Reference:

B. Other information

Results:
Remarks:
Reference:

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species:

Exposure period:
Results: LC_{50} (24h) = ... mg/l
LC_{50} (48h) = ... mg/l
LC_{50} (72h) = ... mg/l
LC_{50} (96h) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Exposure period:
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (..h) = ... mg/l
NOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method: *[*
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

B. Other aquatic organisms

Type of test: static **[ ]**; semi-static **[** x**]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: Mysid shrimp
Exposure period: 96 hr
Results: EC_{50} (24h) = ... mg/l
EC_{50} (48h) = ... mg/l
EC_{xx} (.96h) = 2.3 mg/l
NOEC = <1.3 mg/l
Analytical monitoring: Yes **[x]** No **[ ]** ? **[ ]**
Method: .OECD Guidelines 471 B14 in EC Directive 92/69/EEC
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: 100% acitive ingredient, purity:
Remarks: Solutions of the test material were prepared by dilution with sea water. After mixing and allowing undisloved material to settle, the water soluble faction .was added to two corresponding replicate test vessels. Two control vessels were established containing the same dilution water but no test material. The test concentrations 0, 1.3, 2.2, 3.6, 6, and 10 mg/l were selected based on preliminary test results. Mysids then were added to the

test and control vessels. Test organisms were carefully transferred into the appropriate concentrations of newly prepared vessels at the 24, 48, and 72 hour observation periods. In life observations and water analyses were conducted at 0, 24, 48, 72 and 96 hours.

Following 96-hours of exposure, 60-100% mortality was observed in the three highest concentrations, and 25 and 40% mortality was observed in the two lowest concentrations. The 96-hour LC_{50} was determined to be 2.3 mg/l (1.3-10 mg/l; 95% confidence limits. The 96-hour NOEC was < 1.3 mg/l.

Reliability: (1) Valid without restrictions
Reference: Springborn Laboratories, Inc. Report #89-11-3144 (January 10, 1990)

*4.3 TOXICITY TO AQUATIC PLANTS

Species:
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (h) = mg/l
(Endpoint) EC_{xx} (h) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
open-system **[ ]**; closed-system **[ ]**
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.4 TOXICITY TO BACTERIA

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:
Exposure Period:
Results: EC_{50} (. . . h) = mg/l
EC_{xx} (. . . h) = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[ ]**

Exposure period:
Results: . EC_{50} (..d) = mg/l
(Endpoint) EC_{xx} (..d) = mg/l
NOEC = mg/l
LOEC = mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

(*)4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other *(e.g. field test)* **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (. . . . . h) = ... mg/l
(Endpoint) EC_{xx} (. . . . . d) = ... mg/l
NOEC = ... mg/l
LOEC = ... mg/l
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:
Remarks:
Reference:

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[ ]**
Species:
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} (. . . . . d) = ... mg/kg
(Endpoint) EC_{50} (. . . . . d) = ... mg/kg
EC_{xx} (. . . . . d) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)
Species:

Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

(b)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:
(c)
Species:
Endpoint: Emergence **[ ]**; Growth **[ ]**; Other **[ ]**
Exposure period:
Results: EC_{50} and/or LC_{50} (7d) = ... mg/l
EC_{50} and/or LC_{50}(14d) = ... mg/l
EC_{xx} and/or LC_{xx} (xxd) = ...mg/l
NOEC = ...mg/l
LOEC = ...mg/l
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species:
Endpoint: Mortality **[ ]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[ ]**
Exposure period:
Results: LD_{xx} or LC_{xx} (xxd) = ... mg/kg
NOEC = ... mg/kg
LOEC = ... mg/kg
Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]*

GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: ....., purity: .....
Remarks:
Reference:

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

Results: Substance:
Species or ecosystem studied:
Effects monitored:
Results:
Chemical analysis:
Remarks: *(Information on environmental conditions (e.g. water characteristics: suspended matter, pH, temperature, hardness; soil/sediment characteristics: % organic matter, clay content)*

Reference:

4.8 BIOTRANSFORMATION AND KINETICS

Type: Animal **[ ]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Results:
Remarks:
Reference:

4.9 ADDITIONAL REMARKS

Results:
Remarks:
Reference:

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Value: mg/kg b.w.:
Discriminating dose:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: purity:

Remarks:
Reference:

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
Species/strain:
Exposure time:
Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.1.3 ACUTE DERMAL TOXICITY

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Value: mg/kg b.w.
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]**
LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:
Route of Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time:
Value:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain:
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification:
Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[ ]**; Not irritating **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .

Remarks:
Reference:

5.2.2 EYE IRRITATION/CORROSION

Species/strain:
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification:
Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.3 SKIN SENSITISATION

Type: Human Patch Test
Species/strain: Humans
Results: Sensitizing **[ ]**; Not sensitizing **[x]**; Ambiguous **[ ]**
Classification: Sensitizing **[ ]**; Not sensitizing **[x]**
Method: Shalanski Patch Test
GLP: Yes **[ ]** No **[x]** ? **[ ]**
Test substance: BFGoodrich Material No. 2 (Stalite) , purity: Unknown
Remarks: 25 males and 25 females volunteers were used in this study. 13 of each sex were African Americans and 12 of each sex were Caucasians selected for considerable suntan to facilitate the assessment of depigmentation potential. The test material was applied to identical spots on the backs of the volunteers for 24-hours every other day for 15 applications. Two weeks after the induction period the sites were challenged with the test material for 24-hours. Reactions were evaluated when the patches were removed.

A minimal transitory reaction was noted in 3 males and 4 females; these were considered insignificant and minimal. No depigmentation was noted. The material was considered not to be a primary irritant, fatiguing agent or sensitizer. .....
Reference: Morris V. Shalanski, 1953

*5.4 REPEATED DOSE TOXICITY

Species/strain: Rat/Carworth
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[x]**; No data **[ ]**
Route of Administration: Dietary
Exposure period: 64 weeks
Frequency of treatment: Daily
Post exposure observation period: None
Dose: 2,500, 5,000, and 10,000 ppm
Control group: Yes **[x]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[x]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOEL: Not Identified

LOEL: 2500 ppm

Results: The test material (see concentrations above) was administered to rats (25/sex/group) for 64 weeks. The animals were individually housed and quarantined for 11 days prior to the start of the study. The control group was fed animal chow without the test material. The test material was diluted with peanut oil and then added to the diets to product the desired concentrations. Hematologic evaluations were conducted on 5 rats/sex/group at the initiation of the test and at interval of 3 months throughout the study. Animals were observed for growth. Histopathological exams were conducted on 88 animals which died during the study (14) or were sacrificed at the end of the weeks 51, 56, and 58. Those animals that were sacrificed were representative of the groups with respect to sex and dietary level.

Daily dietary administration significantly retarded growth in females at 2500 ppm and higher. No effect on growth occurred in males at 2500 ppm. Liver enlargement was noted at all concentrations in both sexes. Diffuse hepatic degeneration was observed in all test animals. However, the severity of the liver changes were not treatment-related. The degenerative changes in the liver were described as diffuse cloudy swellings and fatty metamorphosis of the cytoplasm of the hepatocyte. No compound-related hematopoietic changes were observed in any of the test groups.

Method: *[e.g. OECD, other (with the year of publication or updating of the method used)]* .....
.....

GLP: Yes **[ ]** No **[** x **]** ? **[ ]**

Test substance: Compound 3190 , purity: Unknown

Reference: Treon et al. (1957). The Kettering Laboratory, University of Cincinnati

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: *Bacterial reverse mutation assay*

System of testing: *Salmonella typhymurium*, strains TA-1535, TA-1537, TA-98, TA-100 and *Escherichia coli* strain WP2uvrA-

Concentration: 50, 150, 500, 1500, 5000 ug/plate

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[x]**; No data **[ ]**

Results:

Cytotoxicity conc: With metabolic activation: None toxic
Without metabolic activation: None toxic

Precipitation conc: 1500 and 5000 ug/plate

Genotoxic effects:

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[x]**

Without metabolic activation: **[ ] [ ] [x]**

Method: OECD 471 B14 in EC Directive 92/69/eec

GLP: Yes **[x]** No **[ ]** ? **[ ]**

Test substance: Vanlube® SL, purity: .98 %

Remarks: Remarks: The *S. typhymurium* strains were obtained from the University of California (Berkeley) , and the *E. coli* strain was obtained from the British Industrial Biological Research Association. Overnight subcultures of the stock cultures were prepared in nutrient broth and incubated at 37°C for approximately 10 hours. The test material was dissolved in acetone to prepare the test concentrations noted above. Vehicle and positive controls were run in parallel with the test material. The positive controls were as follows:

Non-activation

TA100: N-ethy-N'-nitrosoquanidine (ENNG), 3 µg/plate
TA1535: ENNG, 5 µg/plate
TA1537: 9-aminoacridine, 80 µg/plate
TA98: 4-nitroquinoline-1-oxide, 0.2 µg/plate
WP2uvrA$^-$: ENNG, 2 µg/plate

Activation (10% liver S9)

TA100: 2-Aminoantracene (2AA), 1 µg/plate
TA1535: 2AA, 2 µg/plate
TA1537: 2AA, 2 µg/plate
TA98: 2AA, 0.5 µg/plate
WP2uvrA$^-$: 2AA, 10 µg/plate

A preliminary toxicity study was conducted to select the appropriate dose levels. Five doses of the test material and the vehicle control (acetone) were tested in duplicate. In addition, 0.1 ml of the maximum concentration of the test material and 2 ml of the molten medium were overlayed onto an agar plate. After 48 hours incubation at 37°C the plates were assessed for revertant colonies.

Two experiments were conducted to assess reproducibility. A substance was considered positive if it induce a dose-related and statistically significant increase in mutation rate (at least twice the spontaneous reversion rate) in one or more strains with or without activation. (Note: In the event of two equivocal experiments a third experiment may be used.) To be considered negative the number of induced revetants compared to the spontaneous revertants should be less than two fold at each dose level employed, the intervals of which should be between two and five fold and extend to the limits imposed by toxicity, solubility or up to the maximum recommended dose of 5000 ug/plate. (Note: In this case the limiting factor was the maximum recommended dose.)

No toxicity was observed to any of the strains. Precipitates were observed at 1500 ug/plate and 5000 ug/plate but did not interfere with scoring. No significant increase in the frequency of revetant colonies was recorded in any strain with or without activation, and the responses of the positive controls were satifactory.

Reliability: (1) Valid without limitations

Reference: Safepharm Laboratories Limited, Project No. 860/032, 17 December 1997

B. NON-BACTERIAL IN VITRO TEST

Type:
System of testing:
Concentration:
Metabolic activation: With [ ]; Without [ ]; With and Without [ ]; No data [ ]
Results:
Cytotoxicity conc: With metabolic activation:.
Without metabolic activation:
Precipitation conc:
Genotoxic effects: + ? -
With metabolic activation: [ ] [ ] [ ]
Without metabolic activation: [ ] [ ] [ ]
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*** 5.6 GENETIC TOXICITY IN VIVO**

Type:
Species/strain:
Sex: Female [ ]; Male [ ]; Male/Female [ ]; No data [ ]
Route of Administration:
Exposure period:
Doses:
Results:
Effect on mitotic
index or P/N ratio:
Genotoxic effects: + ? -
[ ] [ ] [ ]
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

5.7 CARCINOGENICITY

Species/strain:
Sex: Female [ ]; Male [ ]; Male/Female [ ]; No data [ ]
Route of Administration:
Exposure period:
Frequency of treatment:
Postexposure observation period:
Doses:
Control group: Yes [ ]; No [ ]; No data [ ];
Concurrent no treatment [ ]; Concurrent vehicle [ ]; Historical [ ]
Results:
Method:
GLP: Yes [ ] No [ ] ? [ ]
Test substance: . . . . . , purity: . . . . . .
Remarks:
Reference:

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[ ]**
Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Exposure period:
Frequency of treatment:
Post exposure observation period:
Premating exposure period: male: . . . . . , female:
Duration of the test:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Parental:
NOEL F1 Offspring:
NOEL F2 Offspring:
Results:
General parental toxicity:
Toxicity to offspring:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity:
Remarks:
Reference:

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

Species/strain:
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Route of Administration:
Duration of the test:
Exposure period:
Frequency of treatment:
Doses:
Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOEL Maternal Toxicity:
NOEL teratogenicity :
Results:
Maternal general toxicity:
Pregnancy/litter data:
Foetal data:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance: . . . . . , purity:
Remarks:
Reference:

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: *(e.g. neurotoxicity, immunotoxicity, etc.)*

Results:
Remarks:
Reference:

B. Toxicodynamics, toxicokinetics

Type:

Results:
Remarks:
References: